The Integration of a Physically-Based Hydrological Model with Spatial Soil Data and GIS: An Application to the Hafren Catchment, Wales

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Declaration

I declare that this thesis has been composed by myself and that it includes only work undertaken by myself, except where explicit reference is made to the work of others.

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a........................... Upslope Drained Area per Unit Contour Length (m^2/m)
BALANCE............ Total Catchment Water Balance
BALEND............ Final Storage in the Root Zone and Unsaturated Soil Column
BALINI .... Initial Storage in the Root Zone and Unsaturated Soil Column
eff .... TOPMODEL efficiency (%)
E_0......................... Potential Evapotranspiration per Unit Area (m/h)
Epot..................... Potential Evapotranspiration per Unit Area (m/h)
Esrz .... Modelled Evapotranspiration per Unit Area (m/h)
m .... Soil Storage-Transmissivity Reçession Parameter (m)
K_0 .... Lateral Saturated Soil Conductivity (m/h)
K_0avg.................. Catchment Averaged Lateral Saturated Soil Conductivity (m/h)
$\ln\left(\frac{a}{T_0 \tan\beta}\right)$ ..... Soil-Topographic Index
q_b .... Subsurface Flow per Unit Area (m/h)
Q_b .... Total Catchment Subsurface Flow (m^3/h)
Q_{INI} .... Catchment Outflow at Beginning of Simulation (m/h)
Q_{obs} .... Observed Catchment Outflow per Unit Area (m/h)
Q_{sim}..................... Predicted Catchment Ouflow per Unit Area (m/h)
q_v .... Saturated Zone Recharge per Unit Area (m/h)
Q_v .... Total Catchment Saturated Zone Recharge (m^3/h)
SBAR .... Catchment Average Soil Moisture Deficit
SBAREND .... Final Storage in the Root Zone and Saturated Soil Zone
SBARINI............ Initial Storage in the Root Zone and Saturated Soil Zone
S_i.......................... Soil Moisture Deficit (m)
SRMAX .... Maximum Root Zone Storage Capacity per Unit Area (m^3/m^2)
SRZ .... Estimated Soil Moisture Content of Root Zone Storage (m)
SUMR .... Total Catchment Rainfall
SUMAE............. Total Catchment Predicted Evapotranspiration
SUMSIM............ Total Catchment Predicted Flows
TEND................. End of simulation period (hrs)
TINI.................... Beginning of module programming
T .... Lateral Soil Transmissivity (m^2/h)
T_0......................... Lateral Saturated Soil Transmissivity (m^2/h)
tanβ .... Tangent of Slope Gradient
γ........................... Catchment Average Soil Topographic Index
ϕ........................... Soil Effective Porosity

List of Acronyms

AWS.............. Automatic Weather Station

BFI................. Baseflow Index Coefficient (HOST Classification)

CIT .... Channel Initiation Threshold (m^2)

CRR............... Conceptual Rainfall-Runoff Modelling

DEM.............. Digital Elevation Model

DTM.............. Digital Terrain Model

GCM.............. Global Climate Modelling

GIS .... Geographical Information Systems \ Geographical Information Science

HOST .... Hydrology of Soil Types

ICM .... Integrated Catchment Management

RDBMS......... Relational Database Management Systems

RS.................. Remote Sensing

SMD .... Soil Moisture Deficit

SPR .... Standard Percentage Runoff Coefficient (HOST Classification)

TIN................ Triangular Irregular Network

TDR............... Time Domain Reflectometry

Abstract

The present research aims to illustrate and evaluate the effect of spatially variable soil data on the modelling of catchment rainfall-runoff transformations, using the hydrological model Topmodel. The soil-topographic wetness index used in Topmodel has always allowed for a spatially variable T_0 – lateral saturated transmissivity – yet very little published research has focussed on the use of spatial soil datasets to derive T_0. In recent years the availability of soil hydrologic parameters, either from soil classifications and/or from new measurement techniques has increased significantly and, especially with regards to remote sensing, there is still great potential for further advances. It is therefore important that models like Topmodel should be able to incorporate such distributed soil data and assess if its' inclusion may allow a better representation of rainfall-runoff transformation processes. In particular, one of the key issues is the need to use distributed data to predict internal catchment conditions – such as runoff source areas – and not only global volumetric outflows. This aspect is of importance both at the catchment scale, for improved integrated catchment management (i.e. in the presence of land-use changes), and at the GCM modelling scale for the simulation of regional land-atmosphere interactions.

With regard to the soil data, particular importance is associated to soil hydraulic parameters such as porosity and saturated conductivities. Traditionally, such data have only been available from measurements on single soil samples. But in recent years, various analytical methods and hydromorphic classification schemes have been developed which allow us to estimate the above parameters or, alternatively, provide qualitative indeces of the soils behaviour in terms of runoff generation. The present research has therefore evaluated the effect of different soil classification schemes with respect to their ability to improve the prediction of soil moisture deficit using TOPMODEL.

Given the strengths of GIS in storing and analysing spatial data, the research has also evaluated if and how GIS can be used to better understand the effect of spatial classification schemes applied to the soil input data. Though GIS cannot substitute the theoretical knowledge of the processes occurring, it can certainly provide the spatial functionalities often lacking in hydrological models. It is this spatial perspective that can allow us to visualise synoptically the phenomena being studied, while at the same time exploring, highlighting, and verifying the prominent spatial variables that control the rainfall-runoff transformation processes.

The integration of the three different modelling perspectives was pursued to allow the user to carry out a more thorough validation of both data and modelling methods used. Ultimately, it is hoped that this multidisciplinary approach will help to better assess the validity of the adopted methodology within the context of integrated catchment management.

Acknowledgements

Possibly one of the better aspects of completing a PhD part-time is the extra amount of time available to build relationships with the many people one comes into contact with, and almost come to know them as friends.

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1. Introduction

The best way to introduce the nature and aims of the present research is to ask a very general question:

Why are hydrological models important?

After all, as Popper has pointed out in his analysis of scientific method (Magee,1973, p. 67), only by asking the right questions can science formulate the procedures to identify better answers. This initial statement may seem excessively theoretical for this research which has concerned itself more with the application of scientific principles than with their review and development, and yet it is of vital importance when considering the possible interaction between hydrology and geographic information science. As in the case of any two scientific disciplines whose proponents decide to interact, there is the inevitable question of who sets the agenda of questions to ask, and therefore of problems to solve. Consequently, by posing the question in terms of hydrological models rather than GIS, I have consciously opted to concentrate on the former. This was not a choice made a priori when the research began, but it has emerged strongly during the various phases, and it is hoped that the reasons why will be apparent in the chapters that follow.

Returning then to the initial question, we can quote from a recent article put forward to define future priorities and objectives for land-surface hydrology.

> ".....Hydrologists are facing important, even fundamental, changes in the direction of their science. New tools, non-traditional datasets, and a better understanding of the connection between hydrology and the rest of the climate system are being developed just as society's needs for improved water management and hazards prediction are becoming critical. ......The continuing shifts in hydrology, driven by new tools and intellectual paradigms, should not take place blindly. The hydrological community must take stock of the current state of knowledge, prioritise the emerging science questions for the coming decade, set objectives, and identify data needs and standards. ......This promise may only be realised if hydrologic data collection and modelling activities are based on sound scientific principles. This is the overall objective of the scientific agenda we propose." (Entekhabi et al., 1999, pg. 2043)

In their statement Entekhabi et al. (1999) touch on the importance of hydrology to society. Events in recent years have underlined how, throughout the world, the impact of man's activities on hydrology (and viceversa) need to be better understood. The growing importance of flood prediction, the need to co-relate land use changes and hydrology and the ability to accurately estimate pollution risks and loads from and into catchments can be taken as some of the more commonly encountered issues.

The prominence of these issues has forced hydrologists and environmental scientists to take a more holistic approach to catchment studies. This has in turn led to an integrated approach to catchment modelling and management, which attempts to understand and reconcile all the different - and often conflicting - aspects of the problems described above..

With regard to the more methodological aspects, Entekhabi et al. (1999) highlight the need of the hydrological research community to come to terms with both new tools and new datasets. But, the authors also stress that the entire process must be based on sound scientific principles. Does this then imply that land-surface hydrological modelling in the past has not been characterised by sufficient scientific rigour?

In recent decades one of the aspects of land-surface hydrology that has continued to receive considerable attention has been that of rainfall-runoff modelling at the catchment scale (Chow, 1964; Anderson and Burt, 1985; Garbrecht, 1987; Singh, 1995). As with other fields within hydrology (e.g. groundwater flow, water quality monitoring, etc.), rainfall-runoff modelling has come to rely on the development of mathematical simulation models, of varying degrees of complexity, capable of predicting the transformation from rainfall to runoff within natural catchments.

These models have evolved rapidly over the past few decades, from simple empirical models to models capable of representing the complex physical and spatial nature of hydrological phenomena (Fleming,1975; Moore et al., 1993). Though the mathematical algorithms of such models can be quite complex, the consideration given to the spatial heterogeneity of processes is not always adequate. This in turn leads to approximations in the results which, if not verified with field validation exercises, can limit the effective validity of the model predictions (Klemes, 1988).

Alongside the development of increasingly complex rainfall-runoff models there has also been a growing awareness amongst the hydrological community, that there is a need

> "to promote the search for an appropriate level of conceptualisation of hydrologic processes compatible with the scale of the phenomena observed on the basin as a whole." (Rodriguez-Iturbe and Gupta, 1983, p.vi)

This awareness has grown stronger in recent years because hydrologists have realised that the acquired theoretical and empirical knowledge of the various processes of the hydrological cycle at the local scale does not lead automatically to the knowledge of how they interact at a higher level (i.e. hillslopes, catchments). The problem of scale is critical for the understanding of hydrological processes, given the multiple spatial and temporal scales that are involved from the hillslope to the global context (Beven, 1995; Engman, 1996).

Furthermore, when examining the equations which represent the processes at the various scales, research has shown that many of the variables involved are specific to the scale at which the analysis is being conducted. This is due to the fact that hydrological processes are always the combined result of processes operating at higher spatio-temporal resolutions (e.g. average soil moisture content is the combined result of local infiltration, capillary rise, etc.) which are integrated over space and time. As a result, both the variables and the physical processes at a given scale may not appear intuitively apparent or interrelated, when viewed from a different scale (Klemes, 1983).

Finally, to the issues mentioned above we can also add that until recently hydrology has been considered by some to be in a transitional state, still evolving into a true science (Klemes, 1986). Consequently the research approach has often been more oriented towards the development of specific problem-solving techniques that provide satisfactory estimates, rather than on understanding the nature of hydrological processes. The inherent risk of this approach lies in the possibility that 'satisfactory results' (for the stated requirements) may be obtained without actually understanding the underlying processes. As Klemes (1986, p. 178S-179S) stated:

> "For a good mathematical model it is not enough to work well. It must work well for the right reason. It must reflect, even if only in a simplified form, the essential features of the physical prototype."

On the basis of these realisations, hydrologists have had to re-evaluate their past approaches and identify new ones. Klemes (1983) identified two directions that researchers should explore simultaneously if the problems outlined above are to be overcome.

a) Better comprehend the relationship between existing theory and empirical data, generally based on local point measurements. This is necessary if new higher level theories of hydrological processes are to be developed.

b) Examine hydrological phenomena directly at the scale of interest (e.g. catchment scale) thus highlighting and understanding the spatial nature of the physical processes. This approach is being made increasingly feasible due to the development of methodologies to capture and represent spatial data, which rely on geographic information systems (GIS) and remote sensing techniques.

Though more than a decade has passed since the above directions were identified, Entekhabi et al. (1999) have re-confirmed their importance by stating:

> "Field experiments need to be conducted to clarify the many complex interactions among soil, vegetation, and hydroclimate. ... Field and modelling studies should be directed towards a more integrated understanding of the genesis and joint evolution of topography, soils, vegetation, and hydroclimate."

An essential component in this integrated understanding is represented by the soils, the importance of which cannot be undervalued. As Houser et al (1998, p 3405) pointed out:

> "soil moisture links the hydrologic cycle and the energy budget of land surfaces by regulating latent heat fluxes"

and soil is also the medium through which hydroclimate and vegetation interact. Yet due to a lack of spatially distributed soil property measurements and also, perhaps, a lack of understanding within the hydrological community, soils are generally not considered in many hydrological models. But with the growing emphasis on regional and global land-surface hydrological modelling, the incorporation of soil properties data has come to be accepted as an essential factor, and some of the relevant research programmes are summarised by Engman (1996).

If soil properties are to be increasingly incorporated within hydrological models, it is important that hydrologists should have access to easily available national datasets. This would avoid the need for lengthy soil sampling studies, or the use of published research data which may not accurately represent the range of properties within a specific catchment. In the UK this objective has been met with the realisation of two national soil datasets. The SEISMIC (Hallett et al, 1995) and HOST (Boorman et al., 1995) soil datasets are both derived from the large amount of soils data gathered for the UK 1:250,000 soil maps (Soil Survey of England and Wales 1983, Soil Survey of Scotland, 1984). While the SEISMIC dataset contains many of the physical parameters which may be of interest within the broader context of environmental modelling, the HOST dataset concentrates only on those parameters which are of use in characterising the rainfall-runoff transformation within each soil type. What remains to be verified is if such datasets can actually improve the predictive capabilities of hydrological models, both with respect to catchment outflow and spatially distributed measurements (eg. soil moisture deficit).

The above paragraphs have indicated how a more integrated understanding of hydrological processes will require greater capabilities to manage spatio-temporal input data. Within this context, information technology has been acquiring a growing role as a tool for supporting modelling and decision making in general, to the point that Abbott has spoken of a new field of hydroinformatics (Abbott, 1993). Concerned with the study of the aquatic environment in the broadest sense, hydroinformatics applies the ever-expanding range of information technologies involving measurement systems, data collection, data storage and data manipulation, and effectively represents a complex interface between two different levels of knowledge. At the lower level we find the raw spatial data (rainfall, elevations, temperature, etc.), while at the higher level we find the derived information (flows, evaporation losses, etc.) obtained through the application of a suitable analysis methodology.

In recent years, significant attention has been given to the possible role that Geographical Information Science (GIS)[1] can play within such an integrated methodology. Though the historical origins of GIS can be traced back to automated mapping (Tomlinson, 1990), the growing need for spatial modelling of physical processes has brought GIS closer to environmental modelling. The degree of interest in integrating the two disciplines is testified by the many international conferences organised on the topic within the last decade (Goodchild et al., 1993; Goodchild et

[1] The term GI Systems is being replaced by GI Science to indicate a transition from a computer-based technology to an established scientific discipline (Goodchild, 1992; Sui and Maggio, 1999). Within the context of this dissertation, and in accordance with the tendency in GIS literature, the two will be used interchangeably.

al., 1996; Kovar and Nachtnebel, 1993; Kovar and Nachtnebel, 1996; NCGIA, 1996). Furthermore, the increasing availability of georeferenced data is allowing hydrologists to work with larger and larger datasets and this will facilitate the adoption of GIS as a tool to better manage and analyse such data. Some examples of the latter can be found in Graham et al. (1999) with regard to the 3 deg, 5 deg and 1/2 min world topographic datasets and Fuller et al. (1994) for the UK Land Cover map.

The issues outlined in the preceding paragraphs represent the general context within which this research has taken place. The underlying belief I have pursued is that there is still a need to evaluate the benefits of incorporating spatial soil data within process-based rainfall-runoff models, and that GIS can contribute to facilitating this integration. In particular, the research will focus on the role of spatial variability of soil hydrological properties and the effect on soil moisture estimation. This can have important implications both at the catchment scale, for improved integrated catchment management, and at the GCM modelling scale for the simulation of large scale land-atmosphere interactions.

Given the strengths of GIS in storing and analysing spatial data, the research will also evaluate whether GIS can help to better understand the physical processes themselves. Though GIS cannot substitute the theoretical knowledge of the processes occurring, it can certainly provide the spatial perspective often lacking in hydrological models. It is this spatial perspective that can allow us to visualise synoptically the phenomena being studied, while at the same time exploring, highlighting, and verifying the prominent spatial and physical variables that influence the hydrological processes.

Though the present research will focus on the analysis of the simulated hydrological processes, and on the specific detailed workings of one model, this is not intended as it's primary or sole objective. Rather, it is hoped that by investigating the problems of integrating hydrological models, spatially variable soil data and GIS a better understanding of the practical implications will be gained. This would represent a contribution towards identifying a modelling procedure that is suited to applications of integrated catchment modelling and management, where the ultimate goal is that of correctly predicting the physical effects under variable catchment conditions. More generally, the present research will aim to address and engage with the methodological issues raised by Entekhabi et al. (1999) and it will also hopefully provide a positive contribution towards addressing society's needs for better management of water resources.

The structure of the present thesis will begin by presenting an overview of the relevant literature in Chapter 2. This review will also identify the specific research topics that are worthy of further examination, and which will be pursued by the present research. In particular, the review will evaluate the different type of modelling approaches available in order to select a model that is considered to be the most suitable for incorporating the spatial variability of soils. The theoretical and practical aspects of the research methodology will be expanded upon in Chapter 3, with particular emphasis on the structure of the chosen hydrological model and the choice of experimental catchments. Chapter 4 will then present the results of the simulations carried out, with a brief description of the key results. An in-depth analysis and interpretation of the results will be carried out in Chapter 5, which will attempt to bring together all of the various results, provide an overall evaluation of the modelling methodology adopted and indicate the areas that still need further examination. The same chapter will also place the results of this research within the wider context of research using distributed hydrological modelling with spatially variable input and output data. The final chapter in this thesis will conclude by summarising the main results of the present research, underlining the implications for hydrology, soil science and GIS.

2. Literature Review

In facing such a complex, multi-faceted field of activity as this research attempts to do, one of the problems to overcome is the need to summarise two different methods of analysis, one related to the spatial properties and the other related to the physical processes that are involved in the natural phenomena being studied. In a preceding work (Ciaccio, 1995), a comprehensive review of GIS and hydrological modelling was carried out in order to evaluate the potential and the limits for integration. In the present work, the research has been extended to encompass spatially variable soil properties and, therefore, it would not be fruitful to limit the literature review only to GIS and hydrological modelling. Consequently, the present literature review will only summarise the major issues discussed in Ciaccio (1995), and focus more specifically on the literature relevant to the aims of this research. In particular, the literature review will evaluate three key aspects:

a) rainfall-runoff models
b) soil properties and soil moisture measurements
c) the integration of hydrological models with GIS

from which will emerge the methodological approach that will be implemented in the successive modelling phase.

2.1 Overview of Rainfall-Runoff models

The second half of the twentieth century has witnessed significant developments in rainfall-runoff modelling. The combination of improved theoretical understanding and advanced computational methods has allowed researchers to consider, ideally, the many controlling factors and the many processes involved in the hydrological cycle. This technical evolution has also been accompanied by an increasing belief in the need to obtain a holistic view of catchment processes, especially in terms of non-point source production of sediments, nutrients and pollution. As a result, hydrologists have been exploring the possibility of developing an integrated approach to modelling of rainfall-runoff processes at the catchment scale.

In this respect we can identify two distinct approaches that have evolved, the "conceptual" and the "physically-based" approach, both of whose development is strongly tied to the evolution in computer technology. We can also identify two distinct classes of models on the basis of how the spatial nature of hydrological phenomena are conceptualised: spatially "lumped" and spatially "distributed" models

(Fleming 1975; Blackie and Eeles 1985; Beven, 1985). In the former, the spatial variability of hydrological phenomena are not explicitly represented. Consequently, variations in vegetation, precipitation, soil properties, etc. are ignored and spatial uniformity is assumed. In the latter, the spatial variability is instead considered explicitly in the modelling procedure. In particular, the spatial variations of the properties that influence the processes are generally represented by dividing the catchment into a discrete number of finite elements, to each of which we associate a set of process parameters. The resulting catchment response is then obtained by integrating the responses of the single elements over a specified time period. Because of the greater process detail represented in distributed models, some authors identify distributed hydrological models and physically-based models as one category (Refsgaard and Abbott, 1996).

In order to better comprehend the conceptual differences and similarities between the two modelling approaches, these will be further examined in the following paragraphs.

2.1.1 Conceptual Rainfall-Runoff Modelling

Within these type of models, often identified by the acronym CRR, the aim is to establish a mathematical relationship that can be used for synthesizing the transformation from rainfall to runoff (Singh, 1995; Anderson and Howes, 1986). This approach is characterised by the identification of functional relationships (linear or non-linear) between the input and the output data. Though there is no precondition placed on the physical significance of the relationships, these models generally attempt to conceptualise actual processes by representing them as a series of storage elements (nodes) and flow transmission routes (links) (Freeze and Harlan, 1969). This apparent simplicity and straightforwardness has contributed to the widespread use of this approach in rainfall-runoff modelling, as testified by Fleming (1975) and Singh (1988).

This approach requires that models be calibrated so as to derive the constants or parameters necessary to define the functional relationships. Calibration procedures are usually based on a comparison of model predictions with observed time series of streamflows, for a given rainfall input. During the calibration, the model parameters are regulated so as to maximise the fit between the two sets of data, where the degree of fit is often evaluated using a regression coefficient. Recent research by Legates and McCabe (1999) has indicated that the traditional correlation-based "goodness of fit" methods may not be appropriate for CRR models, and have illustrated other methods which they believe may be more representative of model performance.

Given that the functional relationships are not necessarily physically based, the same is true for the calibration parameters. The latter can simply be considered as mathematical constants which are dependent on the nature of the system being modelled, but which may not reflect the physical processes actually occurring (Dooge, 1968). To overcome this lack of physical significance more sophisticated CRR models have been developed, which attempt to better represent the complexity of rainfall-runoff transformation processes by spatially distributing the key factors (rainfall, soils, vegetation) (Wang and Chen, 1996). This inevitably makes model calibration much more complicated, given the higher number of parameters that must be determined (Fleming, 1975; Anderson and Howes, 1986). As a result, much research has been done on automatic optimisation techniques, which ideally should be able to identify the absolute or global model optima and the associated parameter set. Unfortunately, it is unlikely that this ideal aim will ever be attained, as a number of authors have pointed out (Beven et al., 1987; Gan and Biftu, 1996). The principal reason for this is the inherently imperfect process representation of CRR models, which use parameters that may be insensitive or intercorrelated. Consequently, the calibration of CRR models still continues to involve a combination of manual and automatic calibration methods (Sorooshian and Singh, 1995).

As CRR models have become more complex, there has also been an increasing risk of creating models containing many parameters of little or no physical significance, but able to reproduce any result required. The very real danger, as was pointed out by Klemes (1986, p. 178S), is that in pursuing the systems[2] approach hydrologists

> "gathered around the systems skylight from which they can see nothing at all have no choice but to conjure up a completely new world of synthetic hydrology composed of linear black boxes....".

This is especially true if we consider what is probably the greatest limit of the CRR approach: that of producing models that lose significance if the nature of the hydrological processes varies. This could occur within a single catchment due to natural or anthropogenic factors or, more generally, if we attempt to transport the model to a different catchment. Consequently, the derived functional relationships

[2] In more recent literature, the definition of conceptual rainfall-runoff models incorporates the previously used "systems approach".

may no longer be valid, thus undermining the validity of any model predictions. But, as pointed out by Abbott et al. (1986a, b), it is precisely in the presence of varying catchment characteristics that the need to predict model parameters is greatest.

2.1.2 Physically-based Approach to Modelling

In the physically-based approach, the primary aim is the represention of the actual physical phenomena involved in hydrological processes (Singh, 1988). The practical applicability of this approach for hydrological prediction is therefore dependent on the ability to understand the processes modelled, rather than simply on the mathematical manipulation of data (Anderson and Howes, 1986).

The physically-based models that are obtained can be considered as a synthesis of the hydrologic cycle, with the physical processes represented through empirically or theoretically derived mathematical equations and physically-based parameters. Ideally, given that all the parameters should be directly measurable in the field and/or can be derived from such parameters, the physically-based approach should not require any model calibration (Beven et al., 1987).

In defining a physically-based model, three key methodological aspects should be considered in relation to the predefined model objectives (Singh, 1988):

1) the choice of input data, which will allow satisfactory prediction of required output data (e.g. what temporal resolution of rainfall data is appropriate for the prediction of hourly peak flows);
2) the choice of model structure and geometry, which will adequately reproduce the key elements of the natural environment in which the observed hydrological phenomena occur, within the constraints of available data (eg. the choice of an appropriate spatio-temporal scale/resolution, capable of representing the desired level of detail in the modelling results);
3) the choice of which physically-based relationships will be adopted and the definition of boundary conditions, which will influence the models' capacity to predict the hydrological characteristics of the modelled processes (eg. if and how rainfall infiltration processes are to be represented).

Upon analysis of these three aspects, it becomes clear that the significant differences between the physically-based and the CRR approach are:

a) the explicit reference to model geometry, due to the fact that physically-based models by definition rely on some kind of spatial discretisation to represent the modelled processes. On the other hand CRR models have generally used lumped representations, though more recent versions of some models have included some form of spatial discretisation, as in the case of the ARNO model (Todini, 1996)

b) the reliance on "physically-based relationships" rather than "functional relationships". Whereas the former are derived from field observations and/or theoretical analysis, the latter are prevalently mathematical and statistical in their derivation.

On the whole, the main difference lies in the fact that for physically-based models the input data, the model structure and the model equations should all be chosen, and validated, on the basis of their physical significance.

Yet for all the ideal advantages of physically-based models, their application has been limited by both theoretical and practical problems. Freeze and Harlan (1969) had already observed:

1) the practical difficulties in obtaining data for all the parameters involved;
2) the difficulty of completely describing by mathematical equations all of the phases of the hydrological cycle, especially with regard to overland flow;
3) the inability to define all the physical boundary conditions, as in the case of soil infiltration properties, therefore making resolution of the complete mathematical equations impossible.

2.1.2.1 The SHE Model

Probably one of the most comprehensive physically-based distributed models designed to date is the SHE - Systeme Hydrologique Europeen (Abbott et al., 1986a, b). The model is the result of a European joint project involving the Danish Hydraulics Institute (DHI), SOGREAH of France and the Institute of Hydrology from the UK. The SHE model is based on the representation of hydrological processes through a spatial discretisation of catchments into superimposed 2D layers of square grid element structures (Fig. 2.1). As such, it represents an example of a physically-based model that lends itself naturally to integration with GIS. Later versions of the model have been developed to better simulate groundwater flows and pollutant transport (SHETRANS - Ewen, 1990) and distributed erosion and sediment yield phenomena (SHESED - Wicks and Bathurst, 1996).

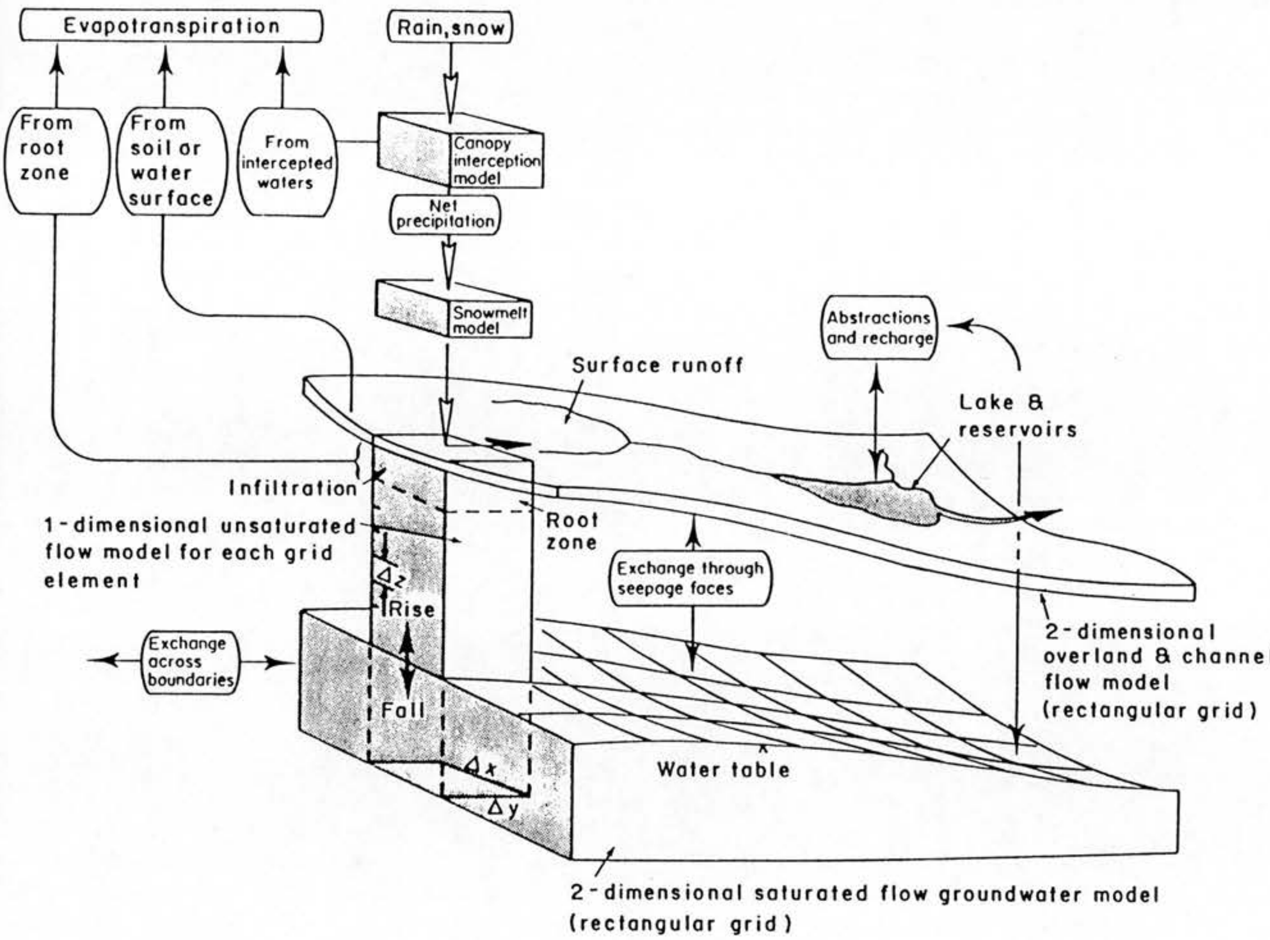

Figure 2.1 – A schematic representation of the structure of the SHE model

(from Beven, 1985)

In developing the SHE model, the authors were aware of the unresolved conceptual problems relating to the spatio-temporal representation of the hydrological processes being modelled (Abbott et al., 1986a, b). In particular, the problem of identifying the theoretical conceptualisation of processes appropriate for a given scale remained unsolved. One possible approach was to develop a conceptualisation of the processes at the catchment scale, in accordance with the views expressed by Rodriguez-Iturbe and Gupta (1983). Instead, the authors decided to adopt an approach which relied on the use of existing empirical and theoretical knowledge of hydrological processes at a more detailed (hydrodynamic) scale. It was therefore assumed that this knowledge could then be used to determine hydrological processes at the desired scale, simply by integrating over space and time.

Yet the authors seem to fall into contradiction with regards to the need to conceptualise hydrological processes at the catchment scale, because they also state that:

> "The full details of all the processes are not needed (and in any case are not yet known). More important is the representation of their gross features, dynamic interaction and collective behaviour at the catchment scale." (Abbott et al., 1986a, p. 51)

This seems to imply that a generalisation - or scaling up - of processes to the catchment scale is nonetheless required. In this respect, Abbott et al. (1986b) and Bathurst (1986a) point out that the large amounts of input data and parameters required will not realistically be available for modelling applications. This therefore raises the question of how the user will identify the parameters capable of representing the aggregate catchment behaviour. In that respect, the authors conclude that the practical use of the SHE will inevitably require the presence of

> "very experienced experts, who set out the different (parameter) scenarios and guide their development through the simulations of historical events." (Abbott et al., 1986a, p. 55)

thus defeating one of the main purposes of physically-based models, that of being easily portable to different catchment conditions. Therefore, while the SHE model is ideally able to synthesise the hydrological processes within the mathematical structure adopted, it cannot but revert to a more conceptual approach in practical applications.

Furthermore, with regards to the grid-based spatial discretisation adopted in the SHE model, Beven (1989) points out that:

1) there is no theoretical basis for assuming that small-scale hydrodynamic theory continues to be valid at the grid scale;
2) the lack of data and of uniformity at the grid scale are incompatible with the assumption of homogeneity (at the grid scale).

Consequently, given that the SHE model relies on the above assumptions being valid, Beven argues that this type of model becomes, effectively, a lumped conceptual model where key spatial input variables are transformed into lumped calibration parameters.

Grayson et al. (1992b) further point out that the scale of homogeneity generally assumed for model elements (10m - 100m) is far greater than that of field measurements but far less than that of the whole catchment. Consequently measured parameter values cannot represent the response of model elements and, also, parameters lose their physical significance because they are no longer representative of field measurements. As pointed out already this leads to the need for calibration of the models, and therefore to the use of effective parameters which are no longer measurable.

The need to calibrate also leads to the limitation that predicted results obtained with the model do not necessarily simulate the processes occurring in all points of the catchment. If, as is generally the case, calibration is carried out on the overall catchment response (e.g. by fitting of predictions to recorded flood hydrographs) there is no theoretical basis to assume that the calibration is valid for processes occurring throughout the catchment (Grayson et al.,1993). The only way in which to validate this aspect would be to carry out field measurements in conjunction with the modelling exercise. This would allow us to verify if the distributed nature of the hydrological processes is being adequately represented in the model structure.

2.1.3 Model Parameterisation

The review of physically-based models has underlined the problem of having to define input parameters at a spatial scale which is much larger than that of field measurements. Until now, the only way to overcome this problem has been to consider 'equivalent' or 'effective' parameter values (Beven 1985; Calver, 1994). These can be considered as values that are representative of the spatially and temporally averaged process characteristics within each model element. But because these parameters are no longer purely physically-based, in the sense of being directly measurable in the field, they are usually obtained through calibration of the model.

The risk associated with calibration is that of detracting from the theoretical rigour of physically-based modelling (Beven, 1985) and thus, at least partially, presenting once again the inherent problem of CRR models. Though the risks of calibration can be minimised by identifying a range of probable parameter values for a given catchment, without appropriate field data there is no way of validating either the significance of the effective input parameters or the models' representation of the physical processes (Beven, 1985). With regard to the latter, an early criticism made by Beven et al. (1987) was that few studies had been carried out comparing model results with internal measurements within the catchment. Without such measurements, Grayson et al. (1992b) point out that there is no way of knowing whether model predictions are realistic, or purely numerical artifacts.

Some proponents of both CRR modelling, such as Wang and Chen (1996), and those of physically-based modelling, such as Bathurst (1986b), advocate that calibration can be based on the interpretation of physical processes. But a strong counter-argument is put forward by Beven when he states:

> "The ability to use physical reasoning in model calibration is not unique to physically-based models and does little to overcome the difficulties of calibrating such models." (Beven, 1989, p.170)

It is the combination of greater requirements for physically-based data, along with the practical need to calibrate physically-based models that has brought about the so-called 'parameter crisis'. This term conveys the conflict arising from the need, on the one hand, for large amounts of data to be input to physically-based models and, on the other, for data that is effectively representative of the variable spatial nature of hydrological processes. The 'crisis' arises from the fact that even if large field measurement campaigns were set up, there would always be some degree of uncertainty (spatial or temporal) associated with the measured parameters (Beven, 1985). This issue has acquired even greater relevance with the extension of catchment scale models to regional or global scales. Research into the issue of spatial aggregation, defined as the spatial averaging of some heterogeneous surface or near-surface variable, has underlined that the method used may be dependent on model formulation (Michaud and Shuttleworth, 1997). Similarily, research into scaling of hydrological processes has concentrated on how the representation of processes is dependent on the modelling scale (Kalma and Sivapalan, 1995).

Though the underlying causes of the 'parameter crisis' have not to date been overcome, recent research has attempted to provide alternative solutions. Probably the simplest and most intuitive approach, but also the most intensive, is described by Wigmosta and Burges (1997). They propose an “adaptive” approach where the measurement and modelling of processes is integrated from the outset of a study. In such a manner, the knowledge acquired from the measurements can aid in better characterising model parameters and, conversely, model results can help identify aspects that need to be better quantified through measurement. Unfortunately, the limit of such an approach is the intensive use of resources (both human and financial), which may not always be available.

The use of sophisticated statistical analyses, such as the Generalised Likelihood Uncertainty Estimation (GLUE) method (Beven and Binley, 1992), or the acquisition of spatial measurements with remote sensing are some of the other directions currently being pursued (Rango and Ritchie, 1996; Georgakakos, 1996) to overcome problems of model parameterisation.

We can therefore conclude that despite significant developments physically-based models have not fulfilled the initial expectations. The view generally held, even by supporters of these models, can be summed up in the following statement:

> "Process-based models are not the panacea they were once thought to be, and it is necessary to be realistic, objective and honest about their capabilities.” (Grayson et al., 1992b, p. 2663)

Only by accepting the limits of physically-based models, can hydrologists go on to use them in a more intelligent manner. When applied with a critical spirit, the advantage of such models is their ability to be used

> "to improve our understanding of processes and their interactions and to identify areas of poor understanding." (Grayson et al., 1992b, p. 2664)

2.1.4 Process Based Hybrid Rainfall-Runoff Models

Following the brief comparison of the CRR and the physically-based approaches, it is obvious that both have their advantages and disadvantages: neither one is the ideal modelling approach. This realisation is not in any way a surprise, as reflected in a statement by Klemes of almost thirty years ago:

"...it makes little sense to argue which of the two approaches is 'better', and to judge the faculties of one by the criteria of the other." (Klemes, 1972, p. 702)

Researchers in the hydrological community have in recent years become aware that the dividing line between the two approaches described is not so clear-cut. In fact, recent developments in hydrological modelling research reflect an attempt to integrate the various approaches (Anderson and Howe, 1986) or, rather, to develop hybrid models that provide a satisfactory compromise between the two approaches (Singh, 1995). Again, it is interesting how this outcome was anticipated thirty years ago:

"It is implicit that the interdependance between physical hydrology and system investigation could lead to the development of a hybrid approach to hydrologic simulation." (Freeze and Harlan, 1969, p. 240)

As far as the theoretical representation of hydrological processes is concerned, Beven (1985) observes that a model should always be seen as an abstraction of reality and, consequently, the physical basis of hydrological processes can never be entirely translated in mathematical terms. It follows from this observation that there is a need to identify aggregated physically-based parameters that can represent the overall nature of the problem and which

"need to retain predictive power at the catchment scale without losing the potential for direct measurement in the field." (Kirkby, 1985b, p.73)

Grayson et al (1992b, p. 2662) in their evaluation of the THALES model have also concluded that:

"The complexity of the natural system is integrated and attenuated in the field, and the challenge is to understand enough of the complexity to develop models that perform a similar integration on model parameters without the need for explicit representation of the underlying complexity."

In this respect, the potential of simpler models that employ a limited number of physically-based parameters has already been highlighted by Anderson and Howe (1986). They refer in particular to the initial work done by Beven and Kirkby (1979) on TOPMODEL, which laid the basis for future research on this type of model.

Interestingly, there has not been much research done comparing and evaluating the different modelling approaches. One of the few reported studies is by Refsgaard and Knudsen (1996) who looked at the following types of models:

a) a spatially lumped conceptual model
b) a semi-distributed hybrid model
c) a fully distributed physically-based model.

It should be noted that semi-distributed models differ from fully distributed ones in the sense that only some of the model parameters are spatially distributed, while others are spatially lumped. Though both may perform equally well in terms of outflow prediction, semi-distributed models may only be able to predict internal states in a simplified form compared to the fully distributed physically-based models. In contrast, the spatially lumped models may not be used to predict internal states within the catchment.

The results of the study by Refsgaard and Knudsen (1996) confirmed that:

- when dealing with ungauged catchments, the semi-distributed model performed better than the physically-based one;
- in the presence of stationary processes and with sufficient measured runoff data (3-5 years) all models compared equally well;
- in the presence of non-stationary processes and with sufficient measured runoff data, all the models were only able to replicate the pattern and magnitude of flows.

These findings, together with those of Michaud and Sorooshian (1994), therefore confirm that in many cases the added complexity of physically-based models is often not justified or required.

Whatever the modelling approach adopted, we should be aware that the choice of which one to implement will be based on (Singh, 1988; Calver, 1993):

a) the specific nature of the hydrological problem;
b) the data availability;
c) the level of accuracy required;
c) the user specifications

In particular, the last aspect must also consider the audience to which the model is aimed (e.g. scientific, public agency, etc.), because this will directly influence both the type of resources available and the user requirements.

The chosen model must also satisfy certain basic requirements. According to Beven (1989, p 158) the model must

> "explore the implications of making certain assumptions about the nature of the real world system"

and also

"predict the nature of the real world system under a set of naturally-occurring circumstances".

We must be able, on the one hand, to use the model to further our understanding of the hydrological processes being modelled and inform our choice of measurement and data collection techniques . But ideally, we must also be able to use the model to predict and forecast runoff events as well as internal catchment states, under varying catchment conditions.

2.1.5 Indices of Hydrologic Similarity

Within the context of hybrid process-based models, the use of hydrological wetness indices has acquired a certain importance, especially for the representation of runoff source areas. According to O'Loughlin (1986) the initial impetus to defining such indices came from the research on the relationship between topography, soils and the existence of saturated runoff generating areas. The idea of a topographic index was initially introduced by Kirkby (1975), who defined it as ($a/\tan\beta$) where a is the upslope area draining through a point, and $\tan\beta$ is the tangent of the slope angle. Beven and Kirkby (1979) later showed how the development of saturated areas was tied to the value of the topographic index, and implemented this in an early version of TOPMODEL. Sometime later, O'Loughlin (1981) used the same concepts to derive a different form of index, which included the effects of topography and soil saturated conductivity. In both cases though, the underlying concept was that:

> "local saturation occurs wherever the drainage flux from upslope exceeds the capacity of a soil profile to conduct that flux." (O'Loughlin, 1986, p.795)

More precisely, the drainage flux from upslope was assumed proportional to the upslope drained area, while the soil flux capacity was assumed proportional to the tangent of the local slope and to the soil transmissivity. This latter parameter was defined theoretically as the integral of the saturated hydraulic conductivity over the depth of the saturated soil profile. This definition therefore allowed the possibility of incorporating spatially variable saturated hydraulic conductivity values, and also of estimating soil moisture conditions.

Based on the above definition, Beven (1986b) re-elaborated the TOPMODEL concepts and defined a soils-topographic index as

$$\ln\left(\frac{a}{T_0 \tan\beta}\right) \quad \text{(Eqn. 2.1)}$$

where T_0 is the soil saturated transmissivity, and introduced a probability distribution function to summarise the spatial variability of the index. In this way, any catchment can be modelled as set of (n) distinct index classes, without having to consider the response of each individual spatial element. This allows the model to account for the spatial variability of the index, without the need to iterate the calculations for each individual spatial element, thus reducing computing requirements. This approach is still implemented in the recent versions of TOPMODEL[3] even though some researchers have begun to question the validity of a single index to represent a wide range of saturation and drydown mechanisms.

In particular, Famiglietti et al. (1998) have carried out field measurements of soil moisture, along a hillslope transect and concluded that:

> "no one predictive index can be expected accurately to predict surface moisture content throughout the entire drydown sequence." (Famiglietti et al., 1998, p.795)

Western et al. (1999) have published the results of a much more extensive study, which measured soil moisture patterns throughout a catchment over a wide range of topographic, aspect and soil conditions. The aims of their study were

1) to verify the presence of spatial organisation in the soil moisture content;
2) to verify how well different types of indices were able to predict the spatial distribution of soil moisture.

Their results are significant in that they have concluded that the ability of a certain index to predict soil moisture distributions depends on the modelling scale, but also on the extent of spatial organisation in the soil moisture distribution. This therefore implies that for any soil classification scheme, the spatial correlation to soil moisture variability may vary throughout the year and is not simply a function of the soil hydrological properties.

Criticism has also been made of the steady-state assumption which underlies both the TOPMODEL and O'Loughlin (1986) wetness indices, which requires that in any point of a catchment, the entire upslope area is contributing to subsurface flow. Research by Barling et al. (1994) and Hemanatha and Wilgoose (1996) has shown

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[3] The model and necessary user documentation can be downloaded from the site http://www.es.lancs.uk/es/research/hfdg/TOPMODEL.html

that this is not always the case. They imply that the subsurface saturated areas may not exhibit spatial connectivity throughout the whole catchment, as TOPMODEL assumes, and that the runoff contributing areas may be varying independently of one another.

Overall though, the research on the use of hydrological wetness indices has contributed significantly towards the development of simplified process-based models that are able to represent the aggregated nature of runoff processes at the catchment scale. Their success can also be gauged by the extent to which they have, to varying degrees, been incorporated in:

1) CRR models such as the ARNO model described by Todini (1996);
2) geomorphological and ecological models (Kirkby, 1997);
3) large scale hydrology models (Nemani et al., 1993; Beven et al., 1995b; Watson et al., 1996);
4) water quality prediction models (Robson et al., 1993).

The use of wetness indices has therefore evolved from their initial purpose of runoff prediction, to that of proxy indices for processes occuring within catchments and for which hydrology is one of the main driving factors. Consequently, researchers are increasingly evaluating how to correctly identify the "most representative" index for predicting specific catchment conditions.

2.1.6 Future Prospects

We have seen how many of the criticisms put forward by researchers that have experimented with physically-based models are accompanied by a desire to go on exploring their potential, convinced of the general validity of an approach that is based on the understanding and representation of physical processes (Beven, 1989). Furthermore Grayson et al.(1992b) underline the need for honest and open discussion on model capability, and criticise researchers' caution in publishing poor model results.

Researchers also recognise that further development is necessary because

> "the collection of data without the benefit of a unifying conception, embodied in a model or theory, may submerge us in an ever deepening sea of seemingly unrelated facts." (Grayson et al., 1992b, p. 2661)

On a more practical level, physically-based models can also aid in the design of field experiments and optimal data collection procedures (Loague and Kiriakis, 1997).

In order to strengthen the validity of physically-based models there are certain fundamental principles that should be implemented. Hillel (1986) lists four of these:

1) parsimony in the number of parameters and in the amount of input data;
2) modesty in the modelling aims;
3) accuracy of prediction in relation to accuracy of measured data;
4) model testability and ability to evaluate limits of model validity.

The recognition of the limits of physically-based models, combined with a firm belief in the need for a sound conceptual framework, has led researchers to explore a third way, that of hybrid process-based models. The four fundamental principles listed above are, in many ways, even more relevant to hybrid models especially in terms of modesty and testability. Furthermore, models based on the use of hydrological wetness indices currently seem to hold greater promise of fulfilling the above principles, unlike the more complex physically-based models.

Though some critics sincerely question whether a new theory capable of explaining catchment scale processes will ever come to be (Smith et al., 1994), it remains a fact that hybrid process-based models have given us a means to question, to interpret and to better understand the complex nature of hydrological processes.

2.2 Soil properties and soil moisture measurements

The importance of soil hydraulic properties in distributed physically-based and hybrid hydrological models cannot be underlined strongly enough. The soil column is the interface between land and atmosphere for all energy-mass transfers (Houser et al., 1998) and therefore controls the complex land-atmosphere feedback mechanisms which characterise the hydrological cycle (Fig. 2.2). Soil parameters such as infiltration capacity, saturated and unsaturated conductivity, as well as porosity, play a fundamental role in the redistribution of water within the soil column. At the same time, from the soil science perspective, it is the movement of water through soils that controls the chemical reactions which influence soil development (Nielsen et al., 1996).

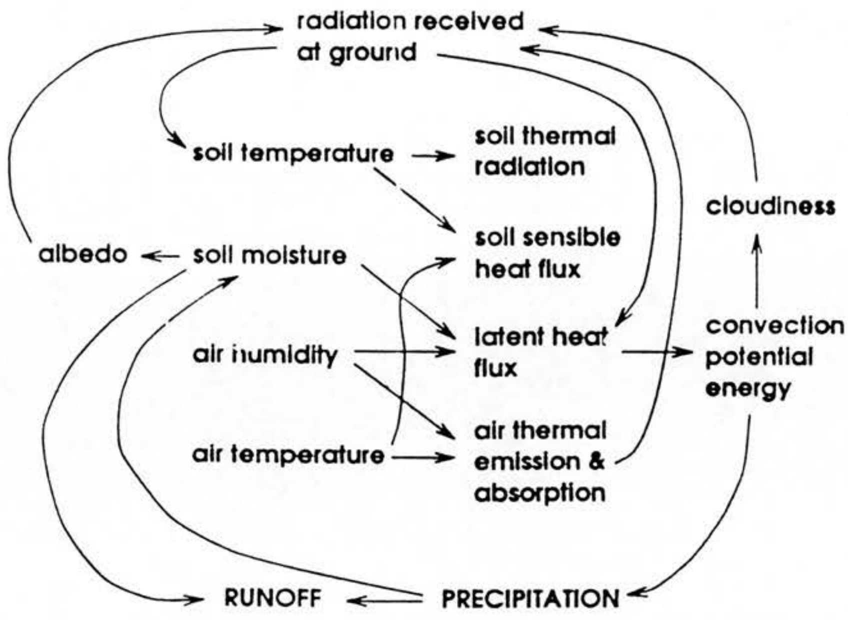

Figure 2.2 – Soil-Atmosphere Interactions
(from Entekhabi et al., 1996)

Generally most hydrological models partition the net precipitation input (rainfall minus interception losses) to the soil into the following components:
- evapotranspiration use by vegetation
- unsaturated storage in the soil matrix
- saturated (groundwater) storage
- lateral throughflow
- surface or overland flow
- baseflow

The ability to correctly model the partitioning will directly affect the simulation accuracy of a chosen model. Furthermore, spatially distributed measurements of soil moisture are important to be able to verify spatial patterns of water accumulation and drainage within a catchment, which are the result of soil moisture gradients. For the above reasons, the methods used to measure the different properties will be briefly reviewed.

2.2.1 Measurement Techniques

The traditional methods used to estimate soil properties and soil moisture content are summarised in Jones(1997) and can be classified as:

- laboratory based;

- in-situ based (permeaters, dip wells, cap. probes, TDR probes, neutron probes,etc.).

Laboratory measurements can be carried out under more controlled conditions and include:

- the gravimetric method which is used for the determination of soil moisture content;
- constant or variable head methods for the determination of saturated soil conductivity.

Yet it is generally quite difficult to obtain undisturbed soil samples, both in terms of water content and pore network, which are also spatially representative (Nielsen et al., 1996). It is therefore often preferable to carry out in-situ measurements.

Tensiometers (Jones, 1997) rely on the equalisation of pressure across a permeable membrane, so that the sensor can measure the pressure in the surrounding soil. These instruments need to operate in relatively wet conditions, due to the risk of air entering the sensor and biasing the pressure readings. Neutron probes (Institute of Hydrology, 1981) rely on the measurement of backscattered gamma radiation, which is proportional to the hydrogen content of the soil. Their main disadvantage, apart from the radiation hazard, is that in the presence of organic soils the sensor will register the presence of hydrogen in the soil as well as in the soil water. Capacitance probes (Dean, 1994) measure the electrical capacitance of the soil, which is a function of the dielectric constant, itself a function of the soil water content. All three methods require calibration if absolute measurements of soil moisture are required. They also present the disadvantages of giving very localised measurements and requiring some disturbance to the soil profile for their installation. For these reasons, time Domain Reflectometry (TDR) sensors have become more common in recent years (Roth et al., 1990). Like capacitance probes, these sensors are based on the relationship between the soil's dielectric constant and the soil moisture content. They present the advantage of sampling a much larger section of the soil profile while requiring minimal disturbance to the soil profile (Rothe et al., 1997).

With regard to saturated or unsaturated soil conductivity and infiltration capacity, infiltrometers and permeaters can be used for in-situ measurements, whereas dipwells and piezometers are used to measure water table depths. The rate of change of water table levels can also be used to estimate vertical and/or horizontal saturated conductivities. It should be pointed out that most soils are not isotropic, and therefore the vertical and horizontal conductivities will be different. Yet due to the difficulties in accurately measuring conductivities in different directions, they are often assumed to be constant.

In addition, the high degree of variability in measurements of saturated conductivity in peat soils poses severe limits to the actual validity of any of the above measurement techniques. This aspect has been highlighted by many authors (Boelter, 1965; Rycroft et al., 1975a, b; Chason and Siegel, 1986; Stunell and Younger, 1995) and, in particular, Rycroft et al. examined whether Darcy's law was actually valid for peats, given that previous research had shown values of saturated conductivity that varied with hydraulic gradient. They concluded that

> "Well humified peat shows departures from Darcian behaviour and it seems necessary to divide peats into two categories with respect to the transmission of water, since Darcy's law can be assumed to apply only to peats of low humification." (Rycroft et al, 1975b, p566)

Another important aspect, for any type of soil, regards the uncertainty and upscaling problems associated with any kind of localised measurement (Nielsen et al., 1996; van Oevelen, 1998). This has led researchers to explore the use of remote sensing techniques to directly measure and/or derive spatially averaged parameters, as well as studying analytical and statistical approaches for determining soil properties.

Remote sensing is considered to be a very promising area of research for the determination of soil properties, and has recently received much attention (Rango and Ritchie, 1996; Georgakakos, 1996). In particular, Engman (1996, p.637) underlines how the developments in remote sensing have been driven by

> "new areas of hydrological analysis; areas where existing methods were unsatisfactory or limiting and areas where sufficient data were sparse or nonexistent. These areas include General Circulation Model (GCM) land parameterisations, advances in snow hydrology, and measurements of soil moisture."

Initial studies focussed on the use of the thermal and infrared band sensors to measure surface temperature, which could then be used to derive soil moisture content (Rango, 1994). Unfortunately, these early approaches did not prove satisfactory due to the inability to separate vegetation effects from actual soil conditions. More recently, significant progress has been made with the use of active and passive microwave sensors. Such sensors are based on the measurement of soil moisture content as a function of the soil dielectric properties. The reasons for the success of such systems are (Jackson, 1996):

a) the ability to operate even through cloud cover and with attenuated sunlight;

b) the ability to measure depth-averaged properties of the soil profile, even though only in the top 0-5 cm.

The main disadvantage of both active and passive microwave systems are (Van Oevelen, 1998)

a) the need to separate the contribution of vegetation moisture

b) the influence of land surface and/or vegetation roughness

c) the influence of soil texture

which lead to the need for complex data interpretation procedures to derive the soil moisture content. As Rango(1998, p. 951) stated:

> "...both active and passive microwave and thermal infrared application need much additional research before they can be used reliably to extract soil moisture information."

Other researchers (Mattikali et al, 1996; Hollenbeck et al., 1996) have also attempted to use remote sensing to determine near-surface soil conductivity as a function of surface drainage rates. While these approaches have clearly identified relationships between soil conductivity and drainage rates for different soils, more research is required before this approach can obtain widespread application.

2.2.2 Analytical and Statistical Methods

Notwithstanding the important progress made in the use of remote sensing, some hydrologists and soil scientists believe that the answer to the problem of spatial measurements of soil properties and moisture is still a long way off. For this reason, they have attempted to develop analytical and statistical methods for the estimation of soil hydrologic properties. One of the earliest attempts was that of Clapp and Hornberger (1978) who derived a general soil classification system based on 11 classes, principally as a function of sand and clay content. The authors also identified two empirical relations for the calculation of conductivity and matric potential:

$$K(\theta) = K_s\left(\frac{\theta}{\theta_s}\right)^{2b+3} \qquad \text{Eqn. 2.2}$$

$$\psi(\theta) = \psi_s \left(\frac{\theta}{\theta_s} \right)^{-b}$$ Eqn. 2.3

where

K_s = saturated conductivity

ψ_s = matric potential at saturation (fitting parameter)

θ = soil moisture content

θ_s = soil moisture content at saturated conditions

b = fitting parameter

On the basis of these two empirical equations, the authors determined fitting parameters for the 11 soil classes they defined, though the approach can be extended to other soil types.

To derive soil saturated conductivity (K_0), Hollis and Wood (1989) have determined empirical regression equations which express K_0 as a function of air capacity. This latter method has been used to calculate saturated conductivity values within the SEISMIC database (Hallett et al., 1995).

An interesting approach to combining remote sensing with the Clapp and Hornberger(1978) classes has been put forward by Simmonds and Burke (1998). Their research attempted to explain the variability in soil radiance as a function solely of water content. The importance of this lies in the fact that past research had concluded that soil radiance depended on the distribution of water within the soil column, which in turn depended on the actual soil structure. Consequently, it could be possible for two similar soils to have the same water content but with completely different radiance values. Simmonds and Burke et al.(1998) have eliminated the soil type variability by identifying statistical functions that, for individual soil classes taken from Clapp and Hornberger(1978), provide a simple relationship between radiance and soil moisture content. If such functions could be identified for a wide variety of soil types, then this approach could certainly represent a significant step forward in the use of remote sensing.

A relatively new direction of research is examining whether it is possible to identify points within catchments, that can actually be considered representative of catchment scale soil moisture conditions (Grayson and Western, 1998). This research draws its justification from the conclusion that, due to the limits of all the measurement methods considered above and also of predictive wetness indices, point measurements of soil moisture are still necessary. The original aspect of the research lies in its' attempt to apply the concept of "time stability" (Vachaud et al., 1985; Kachanoski and de Jong, 1988) to catchments with significant topographic relief. Time stability defines a condition whereby a spatial pattern of soil moisture is invariant over time or, more generally, the statistical relationship between spatial location and soil moisture is invariant over time. This implies that there are points, or areas, of a catchment where the local variations in soil moisture are consistent with the spatially averaged soil moisture variations. If this type of relationship exists, then it would be possible to identify a minimal sampling network that could accurately describe the overall catchment behaviour. In their particular field study, Grayson and Western (1998) used both neutron probes and TDR sensors to measure local soil moisture variations, which were carried out over multiple seasons in three catchments. Their analysis of the measured data is based on the definition for each sampling site of the following parameters.

a) Relative difference in soil moisture content equal to

$$\delta_i = \frac{S_i - \bar{S}}{\bar{S}} \qquad \text{Eqn. 2.4}$$

where: S_i = local volumetric soil moisture content

$\bar{S} = \frac{1}{n}\sum_{i=1}^{n} S_i$ = catchment average volumetric soil content for n sites

b) Mean relative difference for m samples equal to

$$\bar{\delta} = \frac{1}{m}\sum_{i=1}^{m}\delta_i \qquad \text{Eqn. 2.5}$$

From the statistical analysis of the data, the authors concluded that time stable sites that are characterised by a near-zero mean relative difference did actually exist in the three catchments. These sites can therefore be used directly to estimate catchment average soil moisture. Obviously this concept needs to be tested over a wide range of catchments, also in order to develop criteria for identifying time-stable sites. But it has significant potential for providing a valid methodology for extending point measurements to catchment average soil moisture conditions.

Finally, Houser et al. (1998) have advocated the use of data assimilation techniques to integrate the knowledge acquired from remote sensing, ground measurements and hydrological models. Their approach essentially involves using remote sensing and ground measurements to constrain the values of soil moisture to be used as input for a distributed hydrological model. The latter could then be used to estimate the spatial distribution of soil moisture content. Houser et al. (1998) do caution that this type of approach relies on the choice of appropriate statistical analysis methods, which balance the need for maximum amount of input data with that of maximum computational efficiency.

2.2.3 The HOST Classification

In the UK, significant effort has also been put into the Hydrology of Soil Types (HOST) classification (Boorman et al., 1995). This classification was devised in order to provide hydrologists with a source of readily applicable soil hydrologic indeces, that did not require any preliminary interpretation. The classification is based on the schematisation of all soils into three main categories:

a) soils overlying a permeable substrate with a deep acquifer or groundwater table present at depths greater than 2m;
b) soils overlying a permeable substrate with a shallow acquifer or groundwater table present at depths less than 2m;
c) soils overlying a shallow impermeable substrate which restricts vertical water movement and with no significant acquifer.

In the absence of sufficient directly measured soil hydrologic parameters, the classification is based on the following soil properties which were collected for the national soils databases of England and Wales (Soil Survey of England and Wales, 1983) and Scotland (Soil Survey of Scotland, 1984):

a) depth to a slowly permeable layer, defined as having lateral hydraulic conductivity of less than 10 cm/day, which will affect the partitioning between lateral throughflow and vertical percolation in the soil;

b) depth to a gleyed layer, which is considered as an indicator of the frequency of waterlogging within the soil;

c) integrated air capacity, which is a measure of soil macroporosity and is related to hydraulic conductivity in permeable soils and to storage capacity in low permeability and impermeable soils;

d) presence of peaty surface layers, which are capable of storing large amounts of water and have very low hydraulic conductivities;

e) substrate hydrogeology, which is used to distinguish soils that are underlain by acquifers from those underlain by impermeable formations.

The above have been chosen as the key factors which influence the accumulation and flow of water within the soils together with the permeable substrate, if present. On the basis of the above measured factors, the three main soil categories have been divided into eleven conceptual soil response models, which describe the dominant water flow mechanism through the soil (Fig. 2.3). By considering the different possible flow mechanisms within each of the eleven response models, a total of twenty-nine different HOST classes have been identified (Fig. 2.4).

The other input to the HOST classification was the UK national soil map as identified in the 1:250000 soil survey (Soil Survey of England and Wales, 1983; Soil Survey of Scotland, 1984). For any chosen catchment, the percentage of each HOST soil class could be obtained by overlaying the catchment boundary over a 1km gridded version of the UK soil map.

In order to validate the HOST classification, (Boorman et al., 1995) summarise the results of a multiple regression exercise carried out between the Baseflow Index (BFI)[4] coefficient of 575 catchments, and the fraction of HOST classes present in each of the catchments. The multiple linear regression was defined as

$$BFI = a_1 HOST_1 + a_2 HOST_2 + ... + a_{29} HOST_{29} \qquad \text{Eqn. 2.6}$$

where a_i and $HOST_i$ are the regression coefficients and the proportion of HOST classes in the chosen catchment. From the analysis of the 575 catchments, the overall regression coefficient obtained was equal to 0.79. This led the authors to conclude that the HOST classification could be a useful tool in estimating the BFI index for any UK catchment. A similar approach to calculate the Standard Percentage Runoff (SPR) index[5] was adopted . It should be noted that given the limited number of catchments used, equal to 205, the statistical relationship – and therefore the SPR index values of the HOST classes - is not as representative as with the BFI index.

[4] The BFI index was initially developed in the Low Flow Studies programme (Institute of Hydrology, 1980) and is calculated from daily flows as the long-term ratio of baseflow to total flow.

[5] The SPR index was initially developed for the Flood Studies Report (Institute of Hydrology, 1985) and is calculated solely from flood event data. In simplistic terms, it represents the percentage of rainfall that contributes to the quick response runoff (ignoring increase in baseflow).

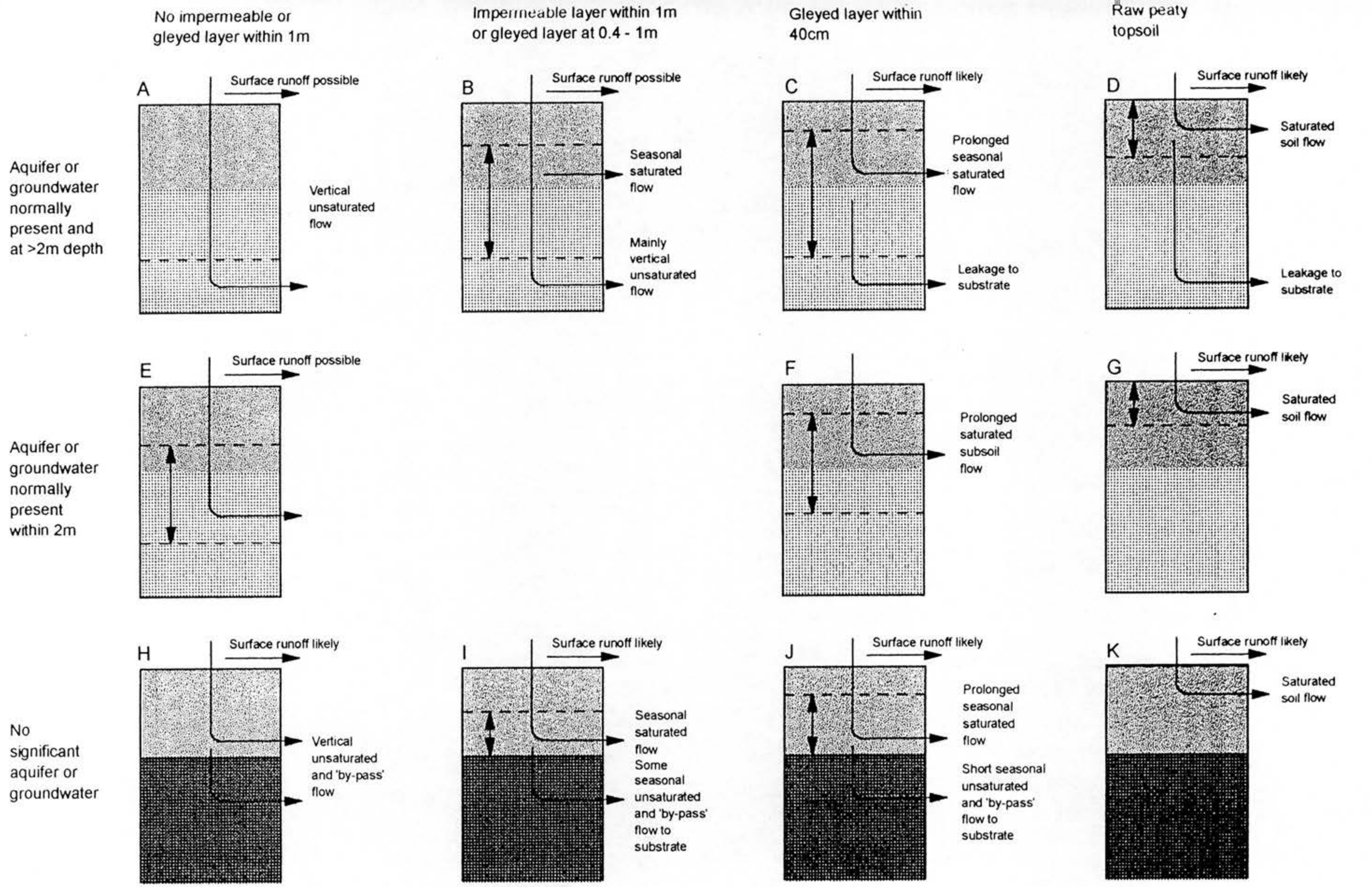

Figure 2.3 – HOST Soil Response Models

(from Boorman et al., 1995)

SUBSTRATE HYDROGEOLOGY	MINERAL SOILS						PEAT SOILS	
	Groundwater or aquifer	No impermeable or gleyed layer within 100cm	Impermeable layer within 100cm or gleyed layer at 40-100cm		Gleyed layer within 40cm			
Weakly consolidated, microporous, by-pass flow uncommon (Chalk)	Normally present and at >2m	1 4.31	13 0.87		14 0.66		15 9.93	
Weakly consolidated, microporous, by-pass flow uncommon (Limestone)		2 2.12						
Weakly consolidated, macroporous,by-pass flow uncommon		3 1.58						
Strongly consolidated, non or slightly porous. By-pass flow common		4 3.33						
Unconsolidated, macroporous, by-pass flow very uncommon		5 5.07						
Unconsolidated, microporous, by-pass flow common		6 2.61						
Unconsolidated, macroporous, by-pass flow very uncommon	Normally present and at ≤2m	7 1.01			IAC* < 12.5 [< 1m day⁻¹]	IAC* ≥ 12.5 [≥ 1m day⁻¹]	*Drained*	*Undrained*
Unconsolidated, microporous,by-pass flow common		8 1.62			9 3.68	10 2.21	11 0.55	12 2.94
			IAC# > 7.5	IAC# ≤ 7.5				
Slowly permeable	No significant groundwater or aquifer	16 0.43	18 5.40	21 4.02	24 13.85		26 2.49	
Impermeable (hard)		17 9.28	19 2.16	22 1.10			27 0.83	
Impermeable (soft)			20 0.69	23 1.31	25 3.64			
Eroded Peat							28 0.58	
Raw Peat							29 5.73	

Small numbers are HOST class number. Large numbers are percentage land cover in England, Wales and Scotland. Also unclassified (urban) areas (5.15%) and lakes (0.74%). No extensive UK soil types exist outside the table or within the shaded portions of the diagram.

* IAC used to index lateral saturated hydraulic conductivity # IAC used to index soil water storage capacity

Figure 2.4 – Summary of HOST Classes

(from Boorman et al., 1995)

2.2.4 Summary of Soil Measurement and Classification Methods

Based on the review of the relevant literature, the following three conclusions can be made on the measurement and classification of soil hydraulic properties.

1) The problem of scale is inescapable for the traditional methods, inasmuch as the point measurement is not necessarily representative of a spatial pattern.

> "The topic of soil moisture and heterogeneity of soil properties clearly requires additional research,.....Finally, there is little question that there is a continuing need for field observations over a range of scales, for validation of models, aggregation schemes, and scaling relationships. These observations should preferably encompass seasonal and inter-annual time scales." (Michaud and Shuttleworth, 1997, p. 180)

2) In the particular case of upland UK catchments, the presence of peats represents a serious drawback insofar as most of the research has focussed on soils in lowland catchments. Also, due to the anisotropy and heterogeneity of organic soils, no method has been identified that is able to give consistent results in the prediction of soil saturated conductivities (Boulter, 1965; Rycroft et al., 1975; Chason and Siegel, 1986). Furthermore, no analytical/statistical methods have been published that can describe the high degree of spatial variability of the hydrologic properties of such soils.

3) Finally, there is the issue of qualitative vs. quantitative soil properties and their use in the validation of distributed hydrological models. There is ample research carried out on the latter, mainly oriented towards process studies. However, there does not appear to have been much research published on the use of qualitative approaches, based on the use of soil hydrological indeces, such as the HOST SPR index previously described. Such approaches could be usefully applied to integrated catchment management, where the user might be more interested in qualitatively evaluating different model parameter scenarios, especially if there is not the scope or resources for collection of field data. Furthermore, under such conditions the appropriate use of GIS and spatial data management and analysis tools becomes an essential component of the modelling exercise.

In all of the approaches described in the previous paragraphs, the most obvious criticism is that any pre-defined classification or statistical relationship will never be able to represent all possible soil types. Nonetheless, it should be noted that only the

HOST classification attempts to predict the hydrological properties of organic soils, while both the Clapp - Hornberger and the SEISMIC approaches effectively ignore the peat formations present in many Northern European catchments (see Moore, 1975). At the same time, the research being carried out on the identification of time stable soil moisture sites within catchments (Grayson and Western, 1998) seems to hold great promise for relating point measurements to areal soil moisture estimates.

2.3 Integrating Hydrological Models and GIS

2.3.1 An Introduction to GIS and Environmental Modelling

In order to understand the implications of integrating hydrological models with GIS, it may be of use to begin by briefly examining the more general aspects relating to the integration of environmental simulation models with GIS. Like hydrological modelling, the broader field of environmental modelling has grown in importance in recent decades. As stated by (Kemp, 1993, p. 107):

> "Environmental issues are among the most important facing decision-makers today. The dynamics of the hydrologic and atmospheric systems of the earth imply that all environmental systems are tightly interrelated, dynamically and spatially. ...Spatial data, systems for managing that data and analytical techniques for converting that data into information are now vital tools in the assessment and management of a healthy natural environment."

As a result of this interest, environmental simulation models have developed as one of the methods capable of furthering our understanding, to the point that today they are considered to be representative of a mature and firmly established field of environmental research (Fedra, 1993; Grayson et al., 1993). The rapid evolution in computer technology has encouraged the development of more powerful environmental simulation models; yet in many of these the spatial dimensions of the phenomena are not explicitly represented (Fedra, 1993).

At the same time, GIS has undergone important developments. These systems have grown from their initial purpose of geographic mapping systems, characterised by a limited number of locational attributes (Tomlinson, 1990), to systems capable of complex spatial data analysis and representation (Peuquet, 1990). The supporting research on spatial data handling has been largely responsible for this evolution and yet, there are still certain conceptual limits that are preventing full integration of GIS with environmental simulation models (Kemp, 1993; Burrough and Frank, 1995; Van Deursen, 1995). This view is supported by the following statements, made by researchers working in both fields

> "Although powerful, GIS-based environmental modelling approaches have characteristics and problems that may constrain their integration." (Moore et al., 1993, p.197)

and

> "GIS and environmental modelling originated in and still represent substantially different domains of expertise" (Parks, 1993, p. 32)

If we examine the fundamental concepts in environmental modelling and GIS we can see that (Fedra, 1993):

- in GIS the basic paradigm relates to the spatial location of objects and/or processes, to which we can associate concepts relating to motion in the spatio-temporal dimension;
- in environmental modelling the basic paradigm relates to the physical states of objects and/or processes, to which we can associate concepts relating to transformation processes in the spatio-temporal dimension.

The complementarity of the basic paradigms is therefore evident, because all phenomena involving a change of physical states are influenced by the location characteristics and vice versa. Consequently, though both approaches can be successfully applied singularly, the possibility of linking or integrating the two types of approaches seems a natural progression, especially if we consider that in many models the spatial characteristics of the simulated processes are inadequately represented (Steyaert, 1993). But what exactly does integration imply? In order to reply to this question, it is necessary to understand the general characteristics of GIS and how they relate to the structure of environmental models.

2.3.2 Basic Concepts of GIS

In a key text on the subject, GIS have generically been defined as:

> "A system of hardware, software, data, people, organisations, and institutional arrangements for collecting, storing, analysing, and disseminating information about areas of the Earth." (Nyerges, 1993, p. 75)

A definition which is more compatible with the view of environmental modellers is the following:

> "The key as to whether or not any particular geographic data handling system is or is not a GIS lies in whether it contains a range of analytical functions for supporting analysis and decision-making as its raison d'etre."(Peuquet, 1990)

These two definitions provide a useful insight into the way the GIS research community sees itself. On the one hand there is the idea of the GIS as an integral part of a larger information system. On the other there is the view of GIS as a spatial analysis tool which is an integral part of a larger modelling environment.

The conceptual representation of space in GIS is also of fundamental importance. In this regard we can identify two dominant views (Kemp, 1993):

1) space can be regarded as made up of distinct objects to which we can associate descriptive information (attributes) regarding themselves and/or the inter-relationship amongst different objects (object model);
2) space can be regarded as a continuum, a physical field, whose properties are functions of space coordinates and, in the case of dynamic fields, of time (field model).

The object and field conceptual models described above correspond to the vector and raster data model respectively. The first of these is based on the representation of geographic objects as combinations of geometric primitives (point, line, polygon), whereas the second is based on the representation of physical fields as regular discretisations of space (pixels, grids, tesselations) (Peuquet, 1990). Greater detail on how these data models are applied specifically to hydrological models can be found in Ciaccio (1995).

Unfortunately, no one model can possibly provide us with all the information we need. As Van Deursen pointed out:

> "The data model is always a simplification of reality, and the choice of a specific data model is determined by the phenomenon studied and the specific questions to be answered. There will always be the need for the description of reality as both a crisp object related description as for the field description." (Van Deursen, 1995, p.50)

With regard to the use of GIS in representing environmental phenomena, Kemp also observes that

> "While many hydrological and other environmental models are based on theories that assume continuity, current GIS data models can only represent continuous phenomena in a variety of discrete data models." (Kemp, 1993, p. 107)

This critique though can equally be made for distributed hydrological models, given that the spatial discretisation implemented is not able to fully represent the spatial continuity of the modelled phenomena. But they can though represent the temporal continuity of processes to a much greater resolution.

Recent research has focussed on the development of new spatio-temporal data models that are capable of explicitly representing the temporal characteristics of spatial data (Langran, 1992; Peuquet and Duan, 1995; Van Deursen, 1995; Egenhofer and Golledge, 1998; Wachowicz, 1999). Attention has also focussed on how the field data model can be improved to provide better representation of spatially continuous variables (Kemp, 1997). But these can still be considered in the initial phases of experimentation, and the GIS research community recognises that more research is required (Sui and Maggio, 1999). Therefore, the spatial paradigm currently adopted in GIS is not able to assimilate the underlying process paradigm of many environmental models, which assumes spatio-temporal continuity of physical processes (eg. Darcian flow, atmospheric dispersion, etc). Though both environmental simulation models and GIS rely on some type of spatial discretisation, only the former have been able to express the complex cause-effect relationships of physical processes. The strength of GIS is instead in its ability to provide a suitable spatial data structure for the storage and graphical representation of model input and output data.

Within GIS, there are some specific types of spatial components that we need to consider in relation to hydrological modelling, such as catchment boundaries, stream channels, subsurface aquifers, etc., each of which can be represented in various ways. If we examine catchments in particular, our representation must deal with the complex nature of these natural systems which exhibit a high degree of spatial heterogeneity and variability. These aspects will be examined in the following paragraphs.

2.3.3 Spatial Discretisation Models

With regards to physically-based and hybrid hydrological models there are various possible approaches to spatial discretisation. Moore et al. (1993) define three types of

spatial discretisations for fully distributed physically-based models, which are also valid for hybrid models:
- grid-based models
- TIN-based models
- contour-based models

As Romanowicz et al. (1993) pointed out, each type of model presents different types of implementation problems. In the following paragraphs, the various types of models will be discussed and their advantages and disadvantages examined.

Grid-based models

Grid-based models use grid digital elevation models (DEMs) as the underlying spatial structure. They are the most widely used because of the ease of digital implementation and the associated computational efficiency. Moore et al. (1993, p. 208) point out that these type of models "provide the most common structures for modern dynamic process-based hydrological models." Examples of some grid-based models are:
- the physically-based SHE surface and subsurface hydrological model (Abbott et al., 1986a, b);
- the physically-based surface runoff and soil erosion model LISEM (De Roo et al., 1996);
- the hybrid TOPMODEL surface runoff model (Quinn et al., 1991).

Moore et al. (1993) also underline some of the disadvantages of grid-based models, such as:
1) they cannot handle abrupt changes in elevation;
2) the computed flow paths are not always realistic and this leads to approximations in the identification of catchment boundaries and channel networks;
3) a variable degree of data redundancy occurs, dependent on smoothness of terrain.

TIN-based models

TIN-based models use a triangulated irregular network as the underlying spatial structure. TINs generally use a given set of known points, chosen so as to identify critical points, such as ridges, peaks, breaks in slope, channels, etc.. The choice of the initial input points also allows the degree of data redundancy to be controlled.

The advantages and disadvantages of TIN-based elevation models, with respect to grid-based models, have been described by various authors (Palacios-Velez and

Cuevas-Renaud, 1992; Maidment, 1993; Moore et al., 1993). In summary, the main advantages of TINs are:

1) a reduced data redundancy when representing smooth terrain;
2) a better representation of abrupt changes in elevation;
3) a greater ease in identifying lines of steepest slope within each element.

On the other hand, the main disadvantages are:

1) an inferior computational efficiency with respect to grid-based models;
2) a greater difficulty in identifying flow paths.

TIN-based models have been developed that are able to automatically extract drainage networks and remove spurious elevation sinks (Guercio and Soccodato, 1996), often by using break-lines to constrain the generation of triangular elements. But the a priori knowledge of topography and the increased computational burden required detracts from the potential advantages.

Contour-based models

Contour-based models use contour DEMs as the underlying spatial structure. The terrain analysis carried out on the DEM divides the catchment into irregular polygons bounded by adjacent contour and streamlines which are grouped together to form flow tubes, as shown in Figs. 2.5, 2.6 (Moore and Grayson, 1991).

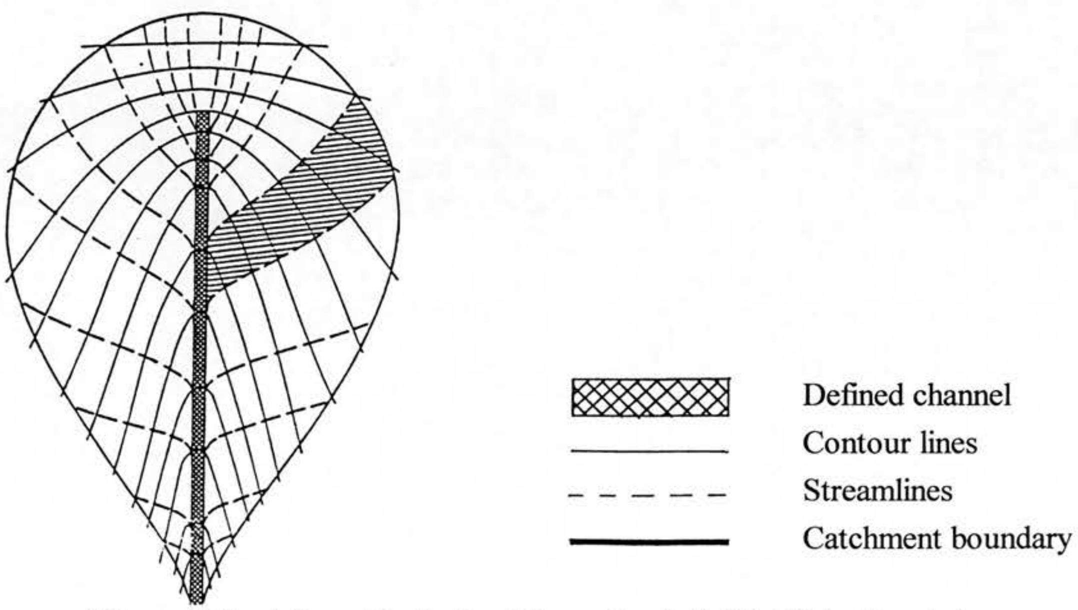

Figure 2.5 – A hypothetical catchment subdivided into flow tubes.
(Moore and Grayson, 1991)

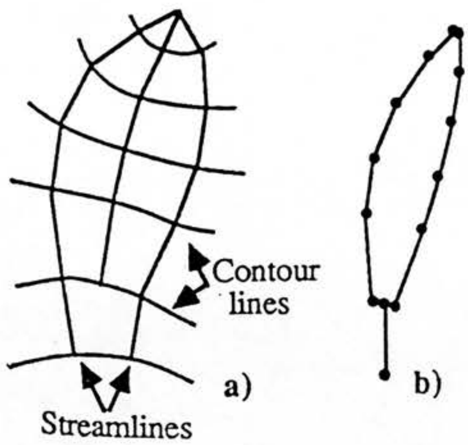

Figure 2.6 – The equivalent one-dimensional network
(Moore and Grayson, 1991)

These models have the advantage of representing the topography in a more natural way in relation to hydrological processes and in explicitly representing flow convergence and divergence. In these models, there is only 1D flow within each element by definition, therefore allowing the process to be represented by a series of coupled 1D equations.

On the basis of their experience developing the THALES model, Moore et al. (1993) believe that the main disadvantage of contour-based models is that of requiring an order of magnitude more data storage for terrain analysis with respect to grid-based DEMs. On the other hand, some criticisms regarding inferior computational efficiency still remain to be fully evaluated.

2.3.4 Evaluation of physically-based parameters

Whatever the spatial discretisation adopted, a critical aspect for all types of process-based models is the evaluation of model input parameters. Moore et al. (1993) consider four general classes of spatial data required:
- topographic data;
- soil data;
- hydrographic data;
- land cover data.

For each of the above classes, the way in which GIS can contribute to parameter identification will be considered.

Topography

When modelling hydrological processes at the catchment scale, gravity is one of the most important driving forces behind the flow of water. The type of topographic data generally required by hydrological models can be divided into primary and secondary attributes (Moore et al., 1993). Primary attributes are calculated directly from a digital elevation model (Tab. 2.1), while secondary attributes are combinations of the primary attributes and represent

> "physically-based or empirically derived indices that characterise the spatial variability of specific processes occurring in the landscape." (Moore et al., 1993, p.201)

Given that terrain analysis techniques are generally included in current GIS, primary and secondary attributes can often be calculated directly within the GIS (e.g. slope, aspect, catchment area, upslope drainage area, etc.).

Attribute	Definition	Hydrologic significance
Altitude	Elevation	Climate, vegetation type, potential energy
Upslope height	Mean height of upslope area	Potential energy
Aspect	Slope azimuth	Solar irradiation
Slope	Gradient	Overland and subsurface flow velocity and runoff rate
Upslope slope	Mean slope of upslope area	Runoff velocity
Dispersal slope	Mean slope of dispersal area	Rate of soil drainage
Catchment slope*	Average slope over the catchment	Time of concentration
Upslope area	Catchment area above a short length of contour	Runoff volume, steady-state runoff rate
Dispersal area	Area downslope from a short length of contour	Soil drainage rate
Catchment area*	Area draining to catchment outlet	Runoff volume
Specific catchment area	Upslope area per unit width of contour	Runoff volume, steady-state runoff rate
Flow path length	Maximum distance of water flow to a point in the catchment	Erosion rates, sediment yield, time of concentration
Upslope length	Mean length of flow paths to a point in the catchment	Flow acceleration, erosion rates
Dispersal length	Distance from a point in the catchment to the outlet	Impedance of soil drainage
Catchment length*	Distance from highest point to outlet	Overland flow attenuation
Profile curvature	Slope profile curvature	Flow acceleration, erosion/deposition rate
Plan curvature	Contour curvature	Converging/diverging flow, soil water content

*All attributes except these are defined at points within the catchment

Table 2.1 – Primary topographic attributes
(Moore et al., 1993)

Soil properties

The traditional representation of soil properties is through the use of choropleth maps that represent the boundaries between different classes. Though this type of representation can be easily transferred to a GIS, it poses two serious problems (Moore et al., 1993):

a) map boundaries have an inherent degree of uncertainty;

b) the assumed homogeneities within each soil class do not exist in reality.

These two factors make it very difficult to use database values as input to physically-based models, even though considerable work has been done to develop national soil datasets, especially in the USA (Lytle, 1993). Furthermore, the soil properties required for hydrological modelling are not always explicitly stored in these databases (e.g. saturated conductivity). This is the case with the US-SCS Curve Number, which is effectively a runoff coefficient (Maidment, 1993). In recent years, soil classification systems like the Hydrology of Soil Types (HOST) (Boorman et al., 1995) and the SEISMIC database of soil properities (Hallett et al., 1995) have significantly increased the amount of easily available data on hydrological properties of soils in the UK. The HOST classification does not provide physically-based soil parameters, but rather coefficients that describe the behaviour of the catchment with regards to baseflow and surface runoff generation. The SEISMIC database instead only provides estimates of soil saturated conductivity for non-organic soils. A similar classification has recently been completed in Australia (McKenzie et al., 2000), based on the soil profile data accumulated for the preparation of the Atlas of Australian Soils.

But even if the soil data are available, there is also a problem of resolution, because as Moore et al. (1993, p 218) stated:

> "The lack of these data at the required spatial resolution is probably the greatest impediment to the successful application of modelling and GIS technologies to analysing resource and environmental problems."

In support of this last point, it is useful to point out that the highest resolution nation-wide soil data is at a scale of 1:12,000 in the USA (Lytle, 1993), whereas in the UK the 1:250,000 soil survey represents the highest resolution data available. If we consider that the most commonly used datasets for hydrological purposes in the UK are the 1:50,000 DEM and river network coverages, it is apparent that the resolution of the national soil survey is inadequate.

Hydrography

The determination of hydrographic parameters is another important problem that affects the integration of hydrological modelling and GIS. There are two different aspects involved: the identification of channel networks and the determination of hillslope drainage flow paths. In both cases the underlying theoretical question is identical: What path does water take through a catchment, from the point in which it falls as precipitation to the outlet? With regard to distributed models this is a critical element given that the flow path will influence both the timing and the magnitude of the flood peaks, as well as the transport of sediments and pollutants.

As far as channel networks are concerned, it is useful to point out that the commonly seen 'blue-lines' drawn on topographic maps are only a representation of the permanently flowing channels, and they may also be subject to a certain amount of subjective judgement (Chorowicz et al., 1992; Moore et al., 1993). This is obviously a source of uncertainty in models, because it has been shown that small

> "first-order streams are a major source of surface runoff in many environments." (Moore et al., 1993, p.206)[6]

Consequently, the misrepresentation of the channel network can often have important effects on catchment flow predictions.

With regard to hillslope flow paths, the problem has been to define hydrologically valid criteria for the accumulation of drainage as water moves downslope. This has important implications for catchment flow predictions given that different computed flow paths are associated with different times of concentration of the flows at the catchment outlet. This in turn will affect both the magnitude and the timing of the flood peaks.

Several automated algorithms have been developed to determine total accumulated drainage area at any point in the catchment, from the analysis of grid DEMs (Band, 1986; Jenson and Domingue, 1988; Fairfield and Leymarie, 1991; Costa-Cabral and Burges, 1994; Nelson and Jones, 1995; Garbrecht and Martz, 1997; Tarboton, 1997). These algorithms determine water flow paths at each point of the catchment, and generally identify channels as those points for which the accumulated drainage area is

[6] Refers to Shreve's classification of channel networks, based on a topological ordering of the single reaches (Shreve, 1966).

above a critical threshold value. When applying such algorithms to DEMs, two important points must be considered.

1) Many are based on the single flow path algorithm of Jenson and Domingue (1988) that does not take into account divergent flow and thus tends to produce unrealistic parallel flow lines along preferential directions (Fig. 2.7). Multiple direction flow path algorithms have been developed, which are better able to represent the dispersive nature of subsurface flow in areas of divergent surface topography (Fairfield and Leymarie, 1991; Quinn et al., 1991, Tarboton, 1997) (Fig. 2.8). But care must always be taken in ensuring that the chosen flow path algorithm correctly reflects catchment flow processes, especially for large catchments where the different types of algorithms may be appropriate in different areas (eg.multiple flow path on hillslopes and single flow path in valley bottoms).

2) It has been shown that the channel initiation threshold (CIT) value used to identify channel networks can be determined either as a constant or as a slope-dependent value. In each case the underlying assumptions have significant implications on the nature of channel initiation processes, as shown by Montgomery and Foufoula-Georgiou (1993). Furthermore, research by Helmlinger et al. (1993) has also underlined the fact that satisfactory criteria for the definition of the most appropriate threshold area have still to be found. The issues regarding the definition of critical thresholds for upslope contributing areas are therefore still the object of on-going research (Quinn et al., 1995; Saulnier et al., 1997a). It is of interest to note that the world river network dataset created by Graham et al. (1999) uses a single threshold area value for all the major world rivers. Yet it is unlikely that surface flow generation within very different catchments can be described solely on the basis of topographic factors alone.

Other researchers have focussed on related topographic issues, such as the extraction of DTMs for flat areas (Garbrecht and Martz, 1997), or the effect of rounding errors (Nelson and Jones, 1995) on flow path algorithms. It is therefore apparent that within the context of rainfall-runoff modelling, there still remains significant scope for research to reduce and quantify uncertainty in the identification of hillslope flow paths and channel networks from DEMs.

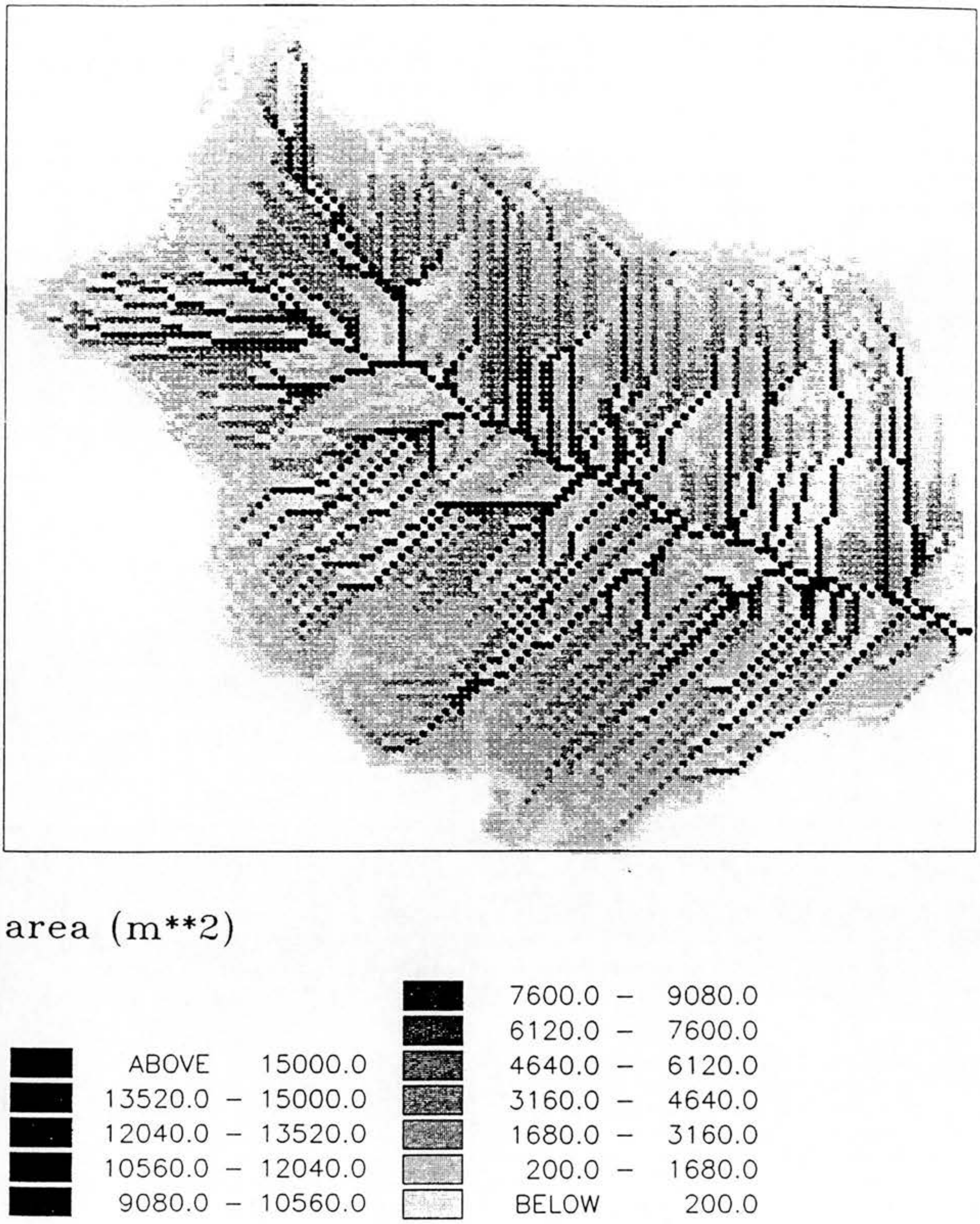

Figure 2.7 – Cumulative map of drained area for single flow path algorithm

(from Quinn et al., 1991)

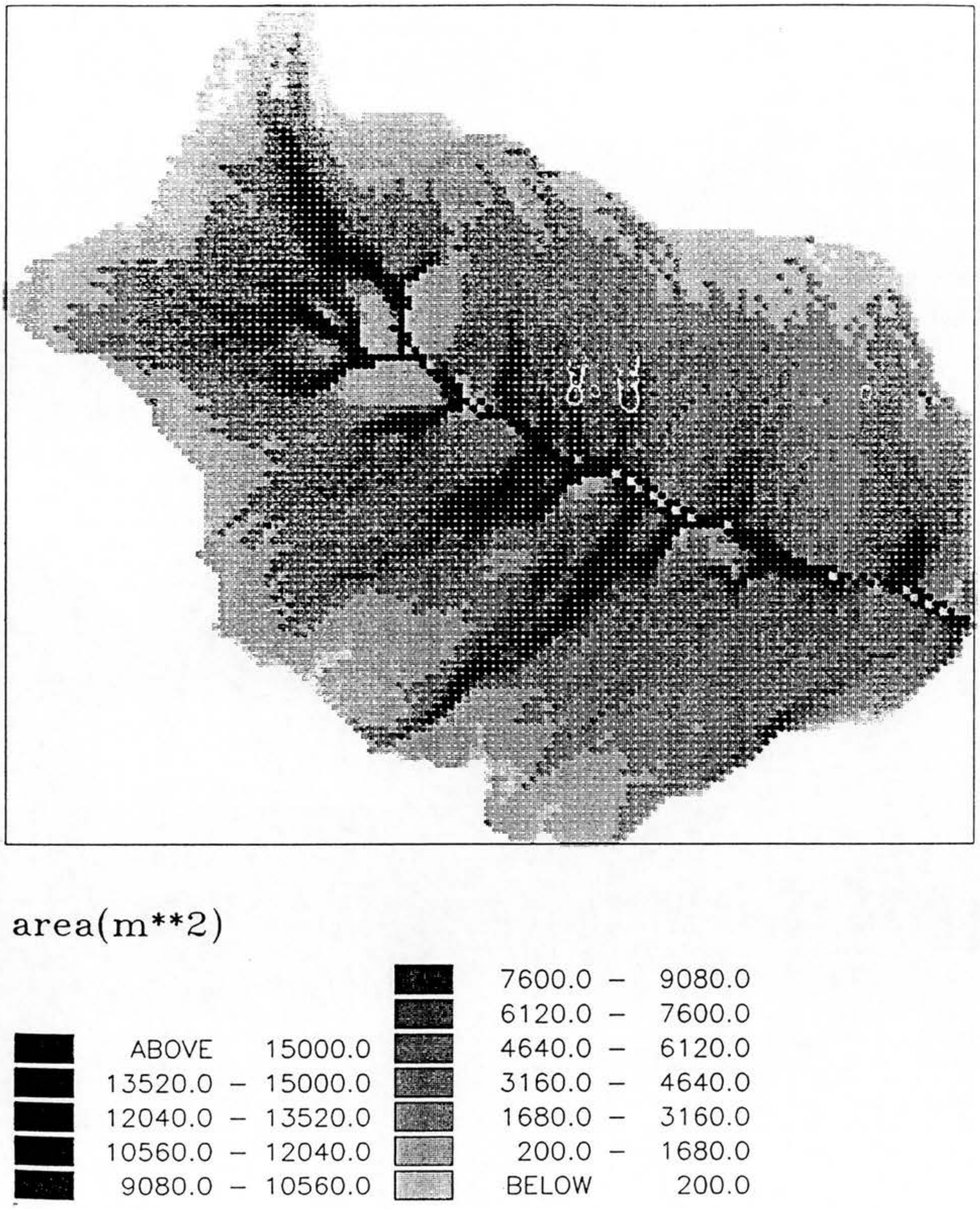

Figure 2.8 – Cumulative map of drained area for multiple flow path algorithm

(from Quinn et al., 1991)

Finally it is important to underline that existing GIS have offered limited hydrological analysis functionalities, as testified by the fact that some of the major packages available contain only the single flow path algorithm (e.g. *flowdirection* command in ARC/INFO GRID, *r.watershed* command in GRASS). This has inevitably restricted the possibility of evaluating flow accumulation input parameters within a GIS.

Land cover

As far as modelling at the catchment scale is concerned, land cover data is important because it can be associated with important input parameters (e.g. interception, evapotranspiration) used in modelling. Land cover data has in recent years become quite easy to obtain, generally by classification of satellite or airborne remote sensing images, of which an important example is represented by the UK Land Cover map (Fuller et al., 1994). RS sensing technologies provide the advantage of time-series of areal data, unlike earth-based sensors which can only provide time-series of point data.

A note of caution in using remotely sensed data regards the inherent uncertainty associated with atmospheric interference with the spectral signal and to errors of interpretation deriving from inadequate ground-truthing (Moore et al., 1993). Once image classification has been carried out, the land cover data and any derived hydrologic surface parameters (eg. interception storage) can easily be stored and manipulated within GIS.

2.3.5 Aims and limits of integration

On the basis of the issues considered in the preceding paragraphs, the different types of integration between hydrological modelling and GIS will now be examined. Essentially, fully distributed process-based models can be supported by GIS in two ways:

- by improving model parameterisation;
- by creating an integrated modelling environment.

Broadly speaking, researchers have identified three levels of integration between GIS and environmental modelling environments (Fedra, 1993; Van Deursen, 1995; Sui and Maggio, 1999), which are briefly reviewed in the following paragraphs and shown in Figs. 2.9, 2.10, 2.11. A summary of the advantages and disadvantages of each type is shown in Tab. 2.2.

In the case of low level integration, the GIS and modelling environments remain distinct and are implemented with existing software packages, each of which has its' own user interface and database structure. For many models, there is actually no database structure for handling input and output data, which are merely stored as ASCII files. What generally occurs is that the GIS is used firstly for the pre-processing of input data to the environmental models, and secondly for the post-processing and visualisation of results predicted by the environmental model.

An example of this type of integration is given by Harris et al. (1993) who point out that while a low-level integration may not be the most elegant, it can certainly aid in the iterative process of model calibration by reducing the time necessary to modify spatial input files. Similarily, Chairat and Delleur (1993) have used a low-level integration between GRASS-GIS and TOPMODEL to calculate some of the model input parameters, specifically the soils-topographic index. Though the authors have made use of GRASS functionalities to calculate some of the model input parameters (e.g. soils-topographic index), they still make use of non-GIS data files input directly into TOPMODEL (rainfall, evaporation, observed flows). Jain et al. (1998) have used a GIS to parameterise the SLURP runoff model but have chosen to calibrate the model flow parameters outside the GIS. Finally the work by Thomas et al. (1999) highlights that, in terms of process understanding, such low-level integration can aid in identifying the principal factors that influence the underlying physical processes.

The conclusions that can be drawn from the above examples of low-level integration are that:

a) it can be a useful approach for identifying the procedural problems to overcome for higher level integration;
b) it can help in improving our understanding of model behaviour, through a more effective visual representation of model results;
c) the GIS is generally not used to calibrate the key model parameters.

The main advantage of using a GIS is the increased ease and speed with which different input datasets can be prepared. This can reduce the time and effort required by modellers to evaluate the effect of different parameters on model performance. Furthermore, the visualisation of model results can highlight inconsistencies in model predictions and thus help the modeller improve the model. On the whole though, the GIS itself can contribute little to furthering the understanding of modelled processes or improving model parameterisation.

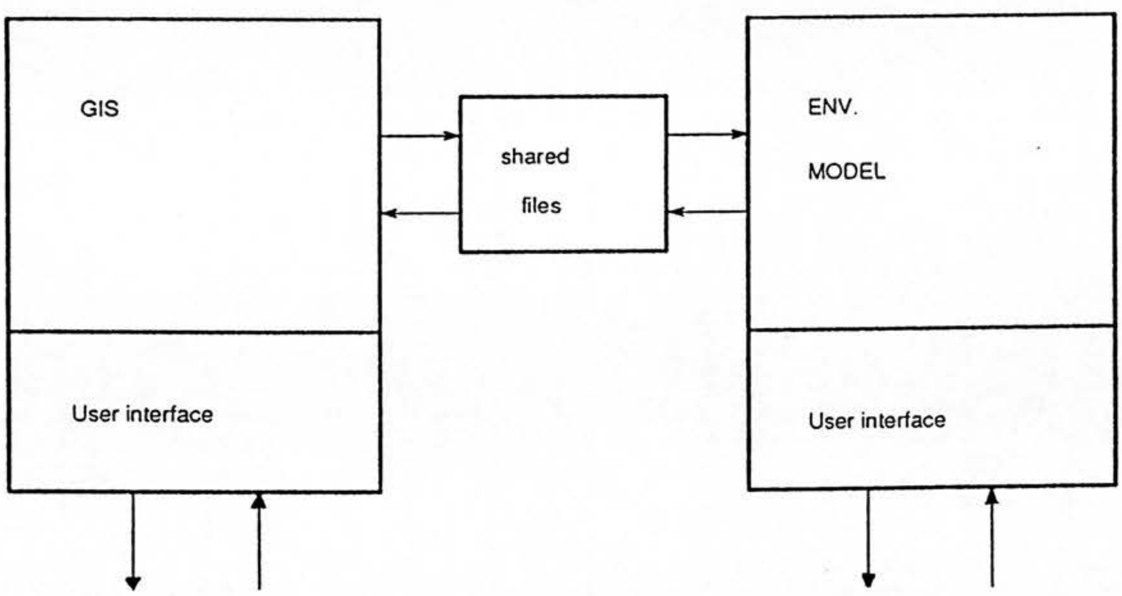

Figure 2.9 – Example of low level integration
(from Fedra, 1993)

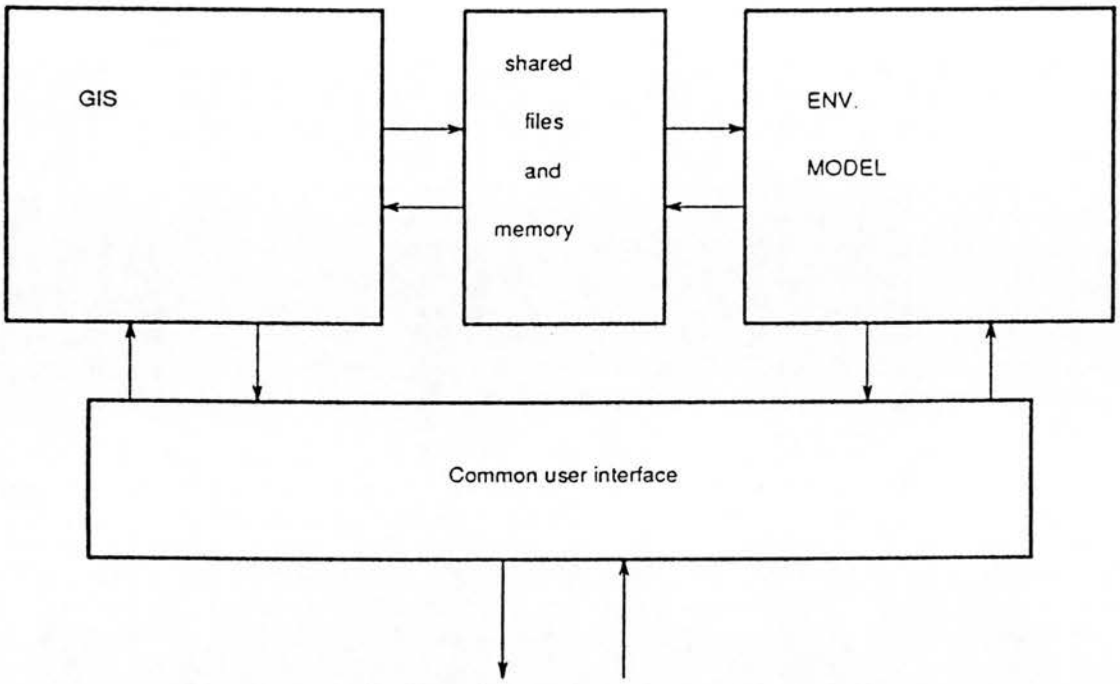

Figure 2.10 – Example of medium level integration
(from Fedra, 1993)

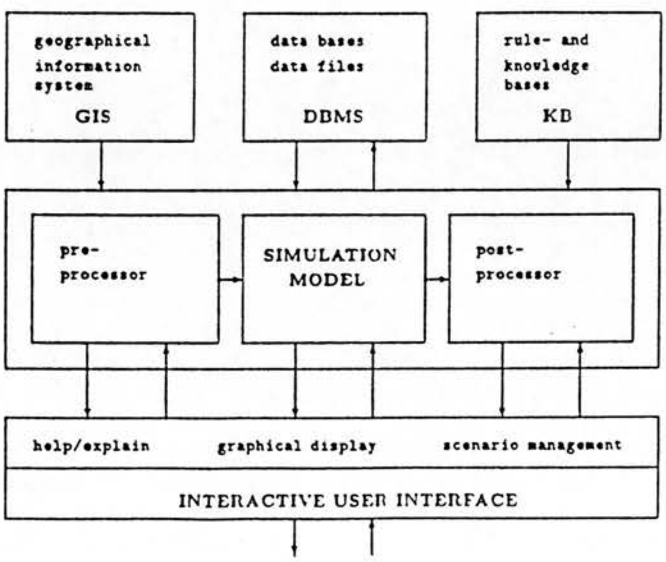

Figure 2.11 – Example of high level integration
(from Fedra, 1993)

Low level integration	advantages	- the development of a low level integration is less time consuming than the development of higher level integration - use of existing programs for GIS and dynamic models yields well known and reliable components for spatial modelling
	disadvantages	- labourious and time consuming - not flexible - error prone because several steps of user interaction are required - new versions of GIS or model require modification of conversion software - redundancy and consistency problems due to the use of several instances of the same database
Medium level integration	advantages	- entire GIS functionality available for manipulation and analysis of input and results of the model - increased speed (no overhead for conversion of data) - easier maintenance of databases, reduced redundancy and consistency problems
	disadvantages	- requires a relatively open GIS structure - low level approach for model formulation
High level integration	advantages	- integration of GIS functionality for manipulation of input, results and formulation of the models - no overhead for conversion between GIS and models and between individual models - rapid development of new models - easy maintenance of models
	disadvantages	- current generation of commercial GIS does not fully support dynamic spatial modelling - investment in development of tools and functionality is high - lack of specialists insight may yield invalid model concepts and formulations, the user is fully responsible for the model formulation

Table 2.2 – The advantages and disadvantages of the three levels of integration between GIS and environmental models

(from Van Deursen, 1995)

In the case of medium level integration, the two approaches are integrated with regard to user functionality and data requirements. Because both the user interface and the data management systems are usually unified, this not only makes the integration more efficient, but it also allows the user to be better guided through the various phases. Nonetheless, the underlying conceptual and logical basis of the environmental model and the GIS remain distinct: the former represents the process component and the latter the spatial component.

Medium-level integration is the least common type found in literature, possibly because it does not have the advantage of simplicity of low level integration, nor that of completeness of high level integration. Gao et al. (1993) offer a detailed description of the approach adopted in interfacing a physically-based hydrological model and the GRASS GIS. The authors offer an interesting alternative as to how GIS can be used when modelling accuracy is limited by the need for excessively large amounts of data. In their case, the linked model-GIS combination can be used as an "investigative tool to target additional data collection and identification of model components requiring improvement." (Gao et al., 1993, p.187). In this context, GIS can therefore support the modelling by offering powerful functionalities that allow the modeller to explore and verify the behaviour of the model with relation to the available data.

Finally, in the case of high level integration the two approaches are fully integrated so that the model becomes simply an application implemented within the GIS or, conversely, the GIS is simply the spatial component of an environmental modelling package (Fedra, 1993).

As an example of high level integration we can consider the work done by Garrote and Bras (1995a), who have developed a Real-Time Interactive Basin Simulator (RIBS) which aims to satisfy the requirements of an integrated modelling, data handling and decision support system. In the particular case of the RIBS system, the modelling is carried out using the DBSIM hybrid model (Garrote and Bras, 1995b) while the spatial data handling and analysis functionalities have been implemented within a tailor-made GIS module.

The advantage of this approach is associated with a unified application environment where ideally:

- the handling and analysis of data is transparent to the user;

- the modelling and/or spatial analysis components are designed to function interdependently, thus allowing the user to more easily test the theoretical basis of the model.

But this approach also presents some serious limitations tied to the fact that:

- the current generation of GIS do not support dynamic process-based modelling;
- the investment needed for the development of these integrated packages is very high.

From the point of view of spatio-temporal data handling and modelling functionalities high level integration represents the ideal solution. Yet an examination of the relevant literature shows that, in many cases, only a low-level integration is implemented. As Fedra (1993, p. 39) pointed out,

> "Linkage with GIS is frequently found, but in the majority of cases, GIS and environmental models are not really integrated, they are just used together".

Especially in the context of experimental research, where the objective is to evaluate different modelling methodologies, it is often not justified or required to implement a high level integration. In that respect, the choice of a low-level integration should not be seen as the simpler solution, but rather as one that allows the researcher to explore and experiment with the functionalities offered by the two environments.

In conclusion, we should remember that when considering the integration of environmental modelling and GIS, the fundamental question that we are attempting to answer is: Can we improve hydrological / environmental models by linking them with GIS? In the preceding paragraphs we have seen how there may be scope for a positive reply to this question, even within the context of a low level integration. The functionalities offered by GIS can allow modellers to:

- better represent the spatial distribution of model input parameters;
- better visualise the multiple spatial scales of modelled processes;
- support environmental models as an exploratory data analysis tool for improving model parameterisation.

With regards to model parameterisation, the objective is the identification of appropriate physically-based parameters (topographic, soil, hydrologic, etc.) through the analysis of model input data (DEM, land cover data, hydrological data, etc.).

Maidment (1993, p.166) has pointed out that:

> "the factor most limiting hydrologic modelling is not the ability to characterise hydrologic processes mathematically, or to solve the resulting equations, but rather the ability to specify the values of the model parameters representing the flow environment accurately."

Yet the review of hydrological modelling literature has clearly shown how process representation and model parameterisation are actually closely interlinked. Consequently, any improvement of spatial functionality within GIS cannot by itself improve model representation of hydrological processes.

As for the future of the integration debate, much will depend on how the two research fields will develop, because as Parks stated the issue is not

> "where new GIS/modelling co-functionality comes to reside, in or out of a GIS or a modelling software environment,..." (Parks, 1993, p.33).

The real issue, and the main challenge for the GIS research community,

> "is to clarify the role of GIS in scientific research and environmental modelling, and to influence the evolution or integration of modelling functionality within the GIS domain." (Goodchild et al., 1993, p. v).

2.4 Future Directions

In looking forward towards new approaches to integrating hydrological modelling, spatially variable soil data and GIS, the present chapter has attempted to identify the key research issues which are crucial to further developments. Several of these have been summarised by Moore et al. (1993) and are listed below:

a) emphasis on identification of physical patterns (eg. saturation) as a function of process;
b) increased support for interactive manipulation of data, and greater ease in data input and output;
c) methods of measuring both data and model accuracy and/or uncertainty;
d) detailed field studies that explore spatio-temporal variability of landscape processes must be continued, also to support model validation;
e) improved mapping of soil hydrological properties.

With regard to the present research, the objective of incorporating spatially variable soil data into a hydrological model is not, of itself, an issue that has never been addressed. But it appears that there has not been significant attention given to how such soil data can be of use in the spatial validation of catchment processes. Considering in particular hybrid process-based models and the concept of partial contributing areas, much research has been carried out on the identification of saturated areas which are responsible for generating overland flow (Beven, 1986; O'Loughlin, 1986). The past research though has essentially considered topography as the only driving factor, ignoring the effect of the soils. It is therefore important to verify whether the incorporation of spatially variable soil properties can lead to better predictions of soil moisture deficit and saturated areas. GIS can also contribute to such research by improving the representation of the spatially variable properties that determine the location and size of these highly dynamic areas. Overall, the integration of the three aspects could lead to a better understanding of the mechanisms of surface runoff generation. Such an understanding would be of use in tackling a wide range of issues - such as water quality, ecohydrology, impact of land use - within the broader context of integrated catchment management (ICM).

Unfortunately, to obtain such results we cannot simply rely on existing modelling and GIS technologies and methodologies. As Grayson et al. (1993) pointed out, problems in catchment management cannot be addressed by the combination of currently available GIS and distributed parameter hydrological models. Rather than striving for a quantitative approach, the authors believe that an alternative approach is required, based on a shift from quantitative predictive capabilities towards "a greater reliance on simple spatial modelling combined with qualitative reasoning" (Grayson et al., 1993, p. 83). This approach would be consistent both with our current understanding and with our ability to represent catchment processes and the data that are available. Grayson et al. (1993) point out that analysing spatially distributed model predictions can be more revealing than looking only at global values, such as total runoff, when assessing model performance. Furthermore, the authors point out the importance of identifying patterns of catchment response as a function of spatial processes. In this way we can verify whether taking into account the spatial heterogeneity of model parameters does result in more accurate model predictions. We can also explore the representation of hydrological processes by a particular model, and validate the spatial predictions against observed data. Within the context of this research, the above approach will be pursued because it seems the most appropriate for investigating the impact of spatially variable soil properties on the prediction of catchment soil moisture conditions.

In this respect, the use of hybrid index based models certainly seems more suited to the above aim, instead of the more complex fully physically-based models. The use of hydrological wetness indices can facilitate the representation of distributed spatial processes, while considering only the key factors that influence catchment behaviour. Though Moore et al., (1993, p. 215) warn that

> "Care must be taken in developing these techniques as simplifying assumptions can introduce rather than resolve computational (and conceptual) complexities."

Grayson et al. (1993, p.90) also recognise that

> "These methods may be no more accurate than complex models but they are much simpler and ...... are 'modest and parsimonious'."

Within the context of a research application, it is the ability of hybrid models to eliminate unnecessarily detailed process representation that makes them so attractive. In particular, the TOPMODEL suite of programs appears to be particularily suited to the spatially distributed prediction of soil moisture conditions in a catchment.

In terms of the choice of soil data and keeping in mind the relevance of this research to realistic ICM type applications, the review of the relevant literature has shown how it would be preferable to use an existing dataset rather than have to carry out catchment specific field-measurements. Soil classifications like HOST or the SEISMIC database therefore seem to represent the best solution and will be further evaluated in the following chapter.

The problem of integrating the hydrological model and the GIS has also been examined and, again for the purposes of a research oriented application, it was felt that a low-level integration would be more appropriate. Even within the context of ICM applications where a higher level of integration may be more suitable, a low level integration can certainly be of use in identifying the key issues to overcome in future developments. Consequently, within the present research GIS will only be used for the pre-processing of model input data and the post-processing and visualisation of model results.

Finally, and most importantly, the literature review presented in this chapter has clearly shown how the problems in integrating hydrological models, spatially variable soil data and GIS have important methodological implications which must always be considered before commencing the actual modelling exercise.

3. Developing a Research Methodology: Theory and Practice

The literature review has highlighted how the integration of hybrid index-based catchment rainfall-runoff models, spatially distributed soils data and GIS still presents various unresolved aspects. Amongst these, the questions the present chapter will consider are listed below.

1) Hybrid index-based models are considered to be more appropriate than physically-based models for modelling distributed runoff processes. But how well are they actually able to represent spatially distributed soil saturation processes within the catchment?
2) Given the difficulty in obtaining spatially representative measures of soil hydraulic properties with the current technology, how can existing datasets of soil hydraulic properties be utilised?
3) What kind of distributed data can be used to validate model results?
4) What should be the role of GIS and what are the limits of GIS for providing the data needed by index-based hydrological models?

In order to reply to the above questions, this chapter will begin by examining the choice of the TOPMODEL model and the underlying theory. It will then go on to consider the choice of field data and the issues of integration with GIS. Finally, it will describe the modifications made to the standard TOPMODEL and describe the modelling procedure which will be carried out.

3.1 The Choice of TOPMODEL

The literature review carried out in the past chapter has presented the reasons for choosing a hybrid index-based model rather than a physically-based one. Within these types of models, much of the published research has originated from the efforts of researchers that have developed TOPMODEL in the UK, and TOPOG in Australia (Vertessy et al., 1994).

In recent years, there has been a significant effort within the TOPMODEL research community to explore the effects of incorporating more spatial variability in the model input parameters[1]. Furthermore, as the following paragraphs will show, TOPMODEL has from the beginning considered soil moisture deficit as an important component in runoff generation processes. Consequently, it made sense to attempt to extend this capability by considering spatially variable soil hydraulic properties. For the above reasons and also because of the practical ease of establishing a dialogue with researchers located closer to Edinburgh, TOPMODEL was selected for the present research.

3.2 TOPMODEL: A Brief History

The TOPMODEL modelling framework is a distributed, physically-based approach based on the hydrological model initially proposed by Beven and Kirkby (1979). TOPMODEL was developed in response to the need

> "for a simple physically-based model for medium sized basins, and, in particular, for a model with parameters that are directly measurable for a given basin." (Beven and Kirkby,1979, p.44)

This would avoid hydrologists having to use parameter values derived from regionalised statistical analyses, especially in ungauged catchments. The application of this latter method, which in the UK culminated in the Flood Studies Report (NERC, 1975), had indicated that the geographic and physical characteristics of catchments could not always be adequately represented with statistical regression methods (Beven, 1986a)[2].

At the same time, previous research had already recognised that the high degree of complexity of catchment systems made it very difficult to represent the large number of physical parameters, even if the hydrological processes were fully understood (Stephenson and Freeze, 1974; Beven, 1989). Consequently the model proposed by Beven and Kirkby (1979) attempted to describe the spatial nature of runoff generating processes while adopting a simplified model structure. A complete description of TOPMODEL theory is given in Beven et al. (1995).

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[1] The culmination of these efforts was the TOPMODEL Symposium held at Lancaster in September 1995, which then led to the publication of Beven (1997).

[2] This observation confirms the inherent limits of the purely conceptual rainfall-runoff approach to hydrological modelling.

It is important to underline the fact that TOPMODEL was initially implemented as a contour-based hydrological model (Beven and Kirkby, 1979; Beven, 1986a). Successively, the procedure has been adapted to a grid-based approach, as described by Quinn et al. (1991) and Quinn and Beven (1993). In the paragraphs that follow, the model structure described is relevant to the grid implementation. For this reason, rather than referring to points in a catchment we will explicitly be referring to pixels, or cells, as the basic spatial element of the model. Furthermore, the model structure described below refers to the basic version provided by the University of Lancaster TOPMODEL group.

3.3 TOPMODEL: Theoretical Background

The model attempts to simulate the distributed effects of hydrological processes by representing the spatial dynamics of saturated runoff generating areas within a catchment. As Quinn and Beven (1993, p.426) stated

> "The model aims to capture the essence of reality while only using three parameters to represent a variety of hydrological phenomena,"

and this allows TOPMODEL to

> "minimize optimisation problems and .... make the final optimised values more physically meaningful."

The theoretical basis of TOPMODEL can be identified in the fundamental assumption that topography is the principal factor that influences the generation and spatial distribution of surface runoff source areas (O'Loughlin, 1981; Beven and Wood, 1983; Wolock and McCabe, 1995). These areas can be identified on the basis of various rainfall-runoff transformation mechanisms which can be classified into four distinct types, as summarised in Fig. 3.1.

a) Infiltration excess overland flow : occurs when rainfall intensity exceeds soil infiltration or storage capacity over all of the catchment, thus producing overland flow (also known as Hortonian flow).
b) Partial area infiltration excess overland flow : occurs when rainfall intensity exceeds soil infiltration or storage capacity on a variable area, thus producing overland flow in parts of the catchment.
c) Saturation excess surface flow : occurs when rain falls over saturated soils with no additional capacity to infiltrate rainfall, thus producing the overland flow component that directly contributes to the storm hydrograph (sometimes also

referred to as lateral subsurface throughflow / quickflow).

d) Subsurface stormflow: occurs when infiltrated rainfall is transformed into fast moving lateral flow in the topsoil. This flow may locally reappear as overland 'return' flow when the soil storage capacity is insufficient.

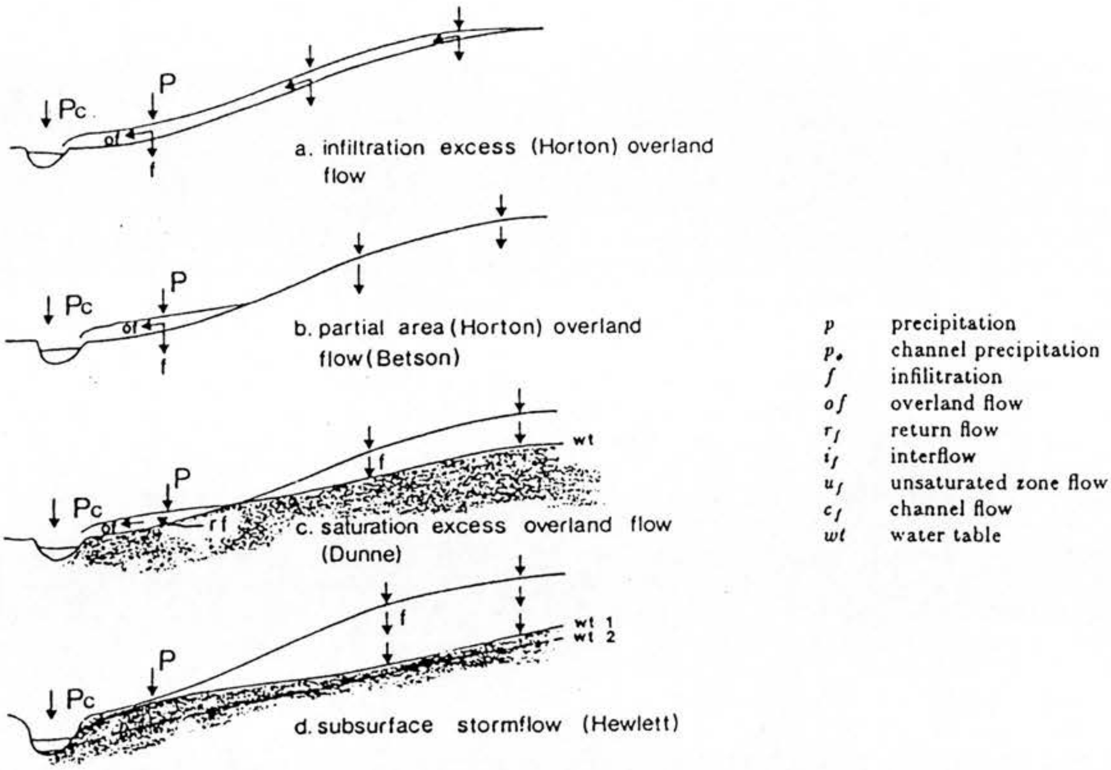

Figure 3.1 - Mechanisms of runoff production

(from Beven, 1986a)

These four classes reflect two conceptual approaches to the formation of surface runoff: an infiltration based approach and a soil storage based approach. Within TOPMODEL, the soil storage based approach has been adopted because it is more physically realistic, at least within the context of humid temperate catchments (Beven and Kirkby, 1979). In this approach, the infiltration rate is not considered to be a limiting factor in runoff generation which is instead assumed to be dependent on the presence of surface saturated areas. Later work carried out on UK catchments has shown how, even in presence of partial area infiltration excess flow, it can be assumed that any of the type A and B flow is re-infiltrated in adjacent areas (Quinn and Beven, 1993). Consequently, TOPMODEL effectively reduces all flow mechanisms to types C and D. These two flow mechanisms are generally considered to be especially valid for upland UK catchments, where the climactic conditions (high levels of precipitation, low temperatures) and the water retention properties of the organic peat soils result in extended periods of near-surface saturation.

The model therefore operates by predicting the three different components that influence runoff generation and recharge to the water table (Beven, 1986a, 1986b):
-saturation excess near-surface[3] flow;
-subsurface storm flow, also referred to as baseflow;
-unsaturated zone drainage to water table, also referred to as saturated zone recharge.

Of these three, the first and the last are predominantly associated with rainfall events, whereas the second component is generated continuously throughout the catchment. Therefore, not only does TOPMODEL simulate the storm runoff component associated with single events, but also the interstorm flow components. By carrying out a distributed water balance at each timestep of the simulation, the model identifies the variable contributing areas of a catchment, from which it then can calculate the various flow and runoff components. The underlying theory for the determination of these different components will be described in the following paragraphs.

3.3.1 Saturation excess surface flow

TOPMODEL assumes that the extent of surface saturated areas, or variable contributing areas, is influenced by the average soil water content throughout the catchment (Beven and Kirkby, 1979). The model accounts for soil moisture variations by conceptualising the catchment as a spatially distributed two component system, comprising the root zone storage and a soil moisture storage (Fig. 3.2). These two storages contribute to the surface and the subsurface flow, as well as to the unsaturated zone drainage to the water table. The soil moisture storage is itself divided into (Quinn and Beven, 1993):

a) an unsaturated zone storage which represents the hydrologically active part of the soil column, within which the flow regime is gravity controlled;
b) a non active storage where water is held in the soil matrix at field capacity and can be considered constant over time.

The model assumes that the root zone storage has to be fully filled before any water will infiltrate into the unsaturated zone storage. This in turn must itself be fully filled before any saturation excess overland flow can occur. It is therefore not sufficient for

[3] In reality, there is often no distinction between overland flow and lateral throughflow in the near-surface soil layer.

the root zone storage to be full, as required by the infiltration excess flow concept; instead the whole soil column must be saturated for surface runoff to take place.

In case of partially filled root zone or unsaturated zone storages, only the precipitation in excess of the volume required to fill them will be transformed into surface flow. Within TOPMODEL, a separate flow component, defined as saturation from above, is calculated in such cases and, together with the saturation excess flow component, makes up the total saturated excess near-surface flow.

For the calculation of soil moisture content within the catchment, TOPMODEL requires the definition of five physically-based parameters.

a) Local slope (ß), which is assumed to approximate the local hydraulic gradient under steady state conditions.
b) Local accumulated upslope area per unit contour length (a), which is considered as a surrogate parameter for the volume of water moving through any given pixel. Moore et al. (1993) have pointed out that even though this condition is only verified under uniform spatio-temporal saturation excess flow, it has been successfully used in other models (e.g. O'Loughlin, 1986, Grayson et al, 1992a; Moore and Grayson, 1991).
c) A parameter (m), which controls the relationship between lateral soil transmissivity and soil moisture deficit (Fig. 3.3).
d) The lateral saturated soil transmissivity (T_0) which can be derived from the lateral saturated soil conductivity (K_0). The model assumes that:

$$T_0 = K_0 m \quad \text{(Eqn. 3.1)}$$

The lateral soil transmissivity (T_i) is the parameter that controls the rate of flow within the soil. It can be expressed as a function of the lateral saturated soil transmissivity (T_0), defined when the water table reaches the surface, and of the local soil moisture deficit (S_i) in the saturated zone:

$$T_i = T_0 e^{(-S_{i=} / m)} = m K_0 e^{(-S_{i=} / m)} \quad \text{(Eqn. 3.2)}$$

A plot of the above equation is shown in Fig. 3.3a, where T_0 is clearly shown as the lateral saturated transmissivity when S_i (soil moisture deficit) is equal to zero.

e) A maximum root zone storage capacity (SRMAX), which is the parameter that controls the evaporation process within the vadose zone.

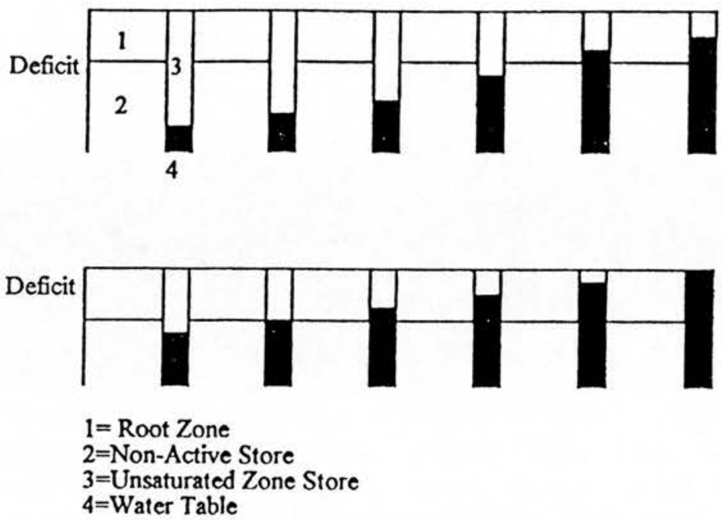

Figure 3.2 - TOPMODEL conceptualisation of soil moisture storages

(from Quinn et al., 1995b)

Figure 3.3 - a) Relationship of transmissivity to soil moisture deficit. b) Relationship between baseflow component and soil moisture deficit

(from Quinn et al., 1995a)

Of these five physically-based parameters the only one that cannot ideally be directly measured or derived, either in the field or from terrain analysis, is the parameter m. It is an effective parameter that controls the

> "rate of the exponential decrease of lateral transmissivity with increasing soil moisture deficit." (Quinn and Beven, 1993, p.428)

The parameter m is physically-based only in the sense that it reflects the global hydrologic response of the catchment storage-transmissivity mechanism (Fig. 3.3). This mechanism controls the recession flow component (baseflow) after surface runoff has ceased (Quinn and Beven, 1993).

A fundamental aspect of the four remaining physically-based parameters is the fact that they all present a high degree of spatial variability. Therefore, given the necessary field and terrain data, all of them could ideally be represented as spatially distributed parameters within TOPMODEL. This is an aspect we will return to in the following paragraphs.

The first three parameters are also used to calculate the so-called *soil-topographic index*

$$\ln\left(\frac{a}{T_0 \tan\beta}\right) \qquad \text{(Eqn. 3.3)}$$

which can be taken as a "theoretical estimate of the accumulation of flow at any point" (Quinn et al., 1995a, p. 162). In particular, it can be considered as an indicator of the tendency of water to accumulate at any pixel in the catchment (through a) and of the tendency for gravitational forces and soil properties to move the water downslope (through $T_0\tan\beta$). High index values indicate a higher probability of soil saturation, due either to large upslope area or to a low flow conveyance capacity of the soil (due to low transmissivities and/or low slopes). Low index values are instead indicative of a lower probability of soil saturation, due either to small contributing area or to a high flow conveyance capacity of the soil. It is further assumed that points with the same index value have a similar hydrological response (Beven, 1997).

One of the fundamental equations of TOPMODEL defines the total saturated flow (q_i) at any given pixel in the catchment as the product of the local transmissivity and local slope:

$$q_i = T_i \tan\beta_i = T_0 \tan\beta_i \exp(-S_i/m) \qquad \text{(Eqn. 3.4)}$$

TOPMODEL assumes that the catchment is always in steady-state conditions, which implies that at each timestep all of the catchment cells are contributing to the total catchment outflow. Under this assumption, the total saturated flow for each cell will be

$$q_i = ra_i \qquad \text{(Eqn. 3.5)}$$

where (r) is the local precipitation intensity and (a_i) is the accumulated upslope area.

By combining equations 3.4 and 3.5, we obtain

$$ra_i = T_0 \tan\beta_i \exp(-S_i/m) \qquad \text{(Eqn. 3.6)}$$

and by separating out the deficit term (S_i)

$$S_i = -m \ln\left(\frac{ra}{T_0 \tan\beta}\right)_i \qquad \text{(Eqn. 3.7)}$$

which allows us to calculate the local soil moisture deficit for a given precipitation[4]. But this equation can be much more useful if it can directly relate the local soil moisture deficit to the average catchment conditions. If we go on to calculate the average soil moisture deficit over the whole catchment (SBAR)

$$SBAR = [\Sigma(S_i\, a_i)] \,/\, \Sigma(a_i) = \Sigma(S_i\, a_i)/A \qquad \text{(Eqn. 3.8)}$$

and substitute equation 3.6 in equation 3.7 to eliminate the rainfall variable (r), we obtain

$$S_i = SBAR + m\left[\gamma - \ln\left(\frac{a}{T_0 \tan\beta}\right)_i\right] \qquad \text{(Eqn. 3.9)}$$

where

$$\gamma = \frac{1}{A}\left\{\Sigma\left[\ln\left(\frac{a}{T_0 \tan\beta}\right)_i a_i\right]\right\} \qquad \text{(Eqn. 3.10)}$$

represents the average soil-topographic index for the catchment. These two equations provide the link between local hydrologic conditions and the average catchment conditions, as summarised by γ. Given that SBAR varies at each time step, it is clear that S_i is a function of time.

As we have seen above, the soil-topographic index is essential for the calculation of

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[4] It is important to note that for TOPMODEL soil moisture deficit is defined with respect to fully saturated soil conditions, whereas often soil moisture deficit is calculated with respect to field capacity.

soil moisture deficits in any pixel in the catchment. But it is also of fundamental importance in determining overall catchment response. One of the most powerful and effective tools in the TOPMODEL approach is the frequency distribution function of $\ln(a/T_0 \tan\beta)$ versus catchment area (Fig. 3.4). Through this distribution function we are able to aggregate all the pixels in the catchment into a discrete number of intervals of $\ln(a/T_0 \tan\beta)$. Within each interval we can assume that all pixels are hydrologically similar and, consequently, pixels belonging to the same $\ln(a/T_0 \tan\beta)$ interval will also have the same value of soil moisture deficit (S_i). All saturated pixels will be those belonging to intervals for which $S_i <= 0$, and the total catchment saturation excess overland flow will be equal to the sum of flows from these pixels.

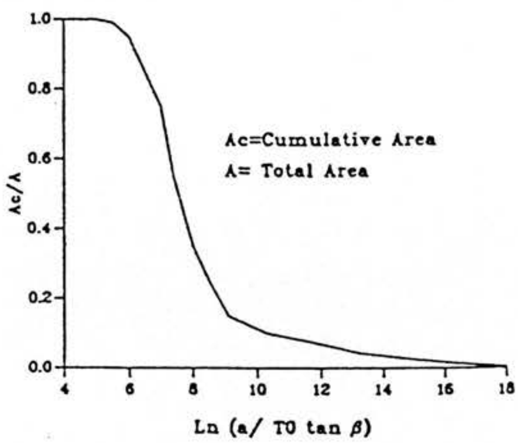

Figure 3.4 - Cumulative frequency distribution of ln(a/T0tanß) versus total area

3.3.2 Subsurface storm flow

In the saturated soil zone, a part of the stored water will contribute to outlet flows as subsurface flow (q_b) which is given by the following equation (Beven, 1986a):

$$q_b = q_o \ \exp(-SBAR/m) \qquad \text{(Eqn. 3.11)}$$

where

$$q_o = \exp(-\gamma) \qquad \text{(Eqn. 3.12)}$$

The constant (q_0) represents the subsurface flow when SBAR=0 which occurs when the average soil moisture deficit over all of the catchment is zero. It should also be noted that q_b represents a flow per pixel, which when summed for all pixels in the catchment gives the total catchment subsurface flow Q_b.

3.3.3 Saturated zone recharge

It is also important to evaluate what proportion of water contained in the unsaturated storage drains to the underlying water table, therefore contributing to incrementing catchment average soil moisture deficit (SBAR) rather than directly to surface runoff. This flow is assumed to be related both to local storage deficit and to local hydraulic transmissivity, through the equation (Beven, 1986a):

$$q_v = \alpha K_0 \exp(-S_i/m) \qquad \text{(Eqn. 3.13)}$$

where (α) is a parameter representing the effective vertical hydraulic gradient. Normally, α is set to one, thus implying that the vertical flux is equal to the saturated hydraulic conductivity (Beven et al., 1995). As with q_b, it should be noted that q_v also represents a flow per pixel, which when summed for all pixels in the catchment gives the total catchment saturated zone recharge Q_v.

3.3.4 Variation of catchment average soil moisture deficit over time

The model simulates the behaviour of the catchment by evaluating, for each time step, the soil moisture deficit (S_i) of each index class. This therefore requires SBAR to be calculated for each time step, as shown by (Eqn. 3.8). In order to do so, TOPMODEL uses a continuity equation whereby the variation in catchment average soil deficit after each time step is given by (Quinn and Beven, 1993):

$$SBAR(t) = SBAR(t-1) + Q_b(t-1) - Q_v(t-1) \qquad \text{(Eqn. 3.14)}$$

where Q_b is the total amount of subsurface flow reaching the channel and Q_v is the total amount of recharge to the water table from the unsaturated zone flows, both of which are summed over the whole catchment.

3.3.5 Evapotranspiration and Interception

The treatment of precipitation losses within TOPMODEL is quite simple. As has already been mentioned, the parameter SRMAX defines the maximum root zone storage capacity. The predicted evaporation is simply assumed to vary linearly with respect to the actual moisture content of the root zone storage, according to the following equation:

$$Esrz = Epot\ (SRZ/SRMAX) \qquad \text{(Eqn. 3.15)}$$

where

- Esrz = predicted evaporation from root zone storage
- Epot = potential evaporation
- SRZ = actual moisture content of root zone storage

It should also be pointed out that because TOPMODEL does not explicitly represent losses by interception, the interception storage is included in SRMAX (Quinn and

Beven, 1993).

The model also accounts for evaporation losses in the presence of saturated soil conditions. This is done in order to reflect a continuous drying of the root zone from the surface downwards, which is important during interstorm periods (Quinn and Beven, 1993).

Calder et al. (1983) carried out an evaluation of different soil moisture deficit models, and concluded that the linear method used in TOPMODEL is usually adequate for UK catchments. The more complex step-function and exponential methods present the disadvantage of requiring additional calibration parameters. Given that for the present study the focus was on evaluating the effects of spatially variable K_0 while maintaining calibration parameters to a minimum, it was decided to only consider the linear model.

3.3.6 Water Balance Calculations

As a means to verify that TOPMODEL has correctly accounted for all the inputs and outputs to the catchment, a final water balance is always calculated at the end of the chosen simulation period, using the following equation:

BALANCE = SUMR-SUMAE-SUMSIM-(BALINI-BALEND)-(SBARINI-SBAREND)

where

- SUMR = sum of total rainfall
- SUMAE = sum of predicted evapotranspiration
- SUMSIM = sum of simulated flows
- BALINI = initial storage in the root zone and unsaturated soil column
- BALEND = final storage in the root zone and unsaturated soil column
- SBARINI = initial storage in the root zone and saturated soil column
- SBAREND = final storage in the root zone and saturated soil column

Over the hydrological year, and in the absence of deep groundwater inputs or outputs, the balance should ideally be equal to zero. However, it is not always possible to establish the presence and contribution of deep acquifers within a catchment.

This may be particularily true for single flood events associated to periods of the year when the flows exchanged with the acquifer may become significant. Examples of this are during periods of snowmelt when the acquifer may be recharged, or extended dry summer periods when the acquifer may experience depletion. In such cases, the balance will not be zero, and its' negative or positive value will give an indication of actual volumes of groundwater released or stored during the event.

Alternatively, it may also be possible that for single events TOPMODEL incorrectly predicts the timing and volume of the simulated flows. In such cases an overestimate of the flows will lead to a negative balance, while an underestimate of the flow will lead to a positive balance and such values will represent a model error.

3.3.7 Model Performance

When quantifying how well any model is able to reproduce measured runoff events, various methods can be used. In TOPMODEL's case, an efficiency criterion is used based on the following equation:

$$eff(\%) = \left\{ 1 - \frac{\sum_{TINI}^{TEND} \left[(Q_{obs}) - (Q_{sim}) \right]_t^2}{\sum_{TINI}^{TEND} \left[(Q_{obs}) - (Q_{avg}) \right]_t^2} \right\} * 100 \qquad \text{(Eqn. 3.16)}$$

where the numerator and denominator in the equation represent the variance of the residual errors and the variance of Qobs respectively, and

$$Q_{avg} = \frac{\sum_{TINI}^{TEND} \left[(Q_{obs}) \right]}{(TEND - TINI)} \qquad \text{(Eqn. 3.17)}$$

is the observed mean flow over the simulation period.

The ideal condition, when the simulated and observed flows match perfectly, yields an efficiency value of 100. But it should be noted that the equation can also provide negative efficiencies. In such cases, the variance of the residual errors in the simulated flows is greater than the variance of the observed flows. In other words, the predicted flows are affected by an error which is greater than the range of variability in the observed flows therefore making any result meaningless.

3.3.8 Derivation of model parameters

Having described the theoretical basis of TOPMODEL, we will now go on to examine how the model parameters are derived. Of the five input parameters required by the model (tanß, a, T_0, m, SRMAX), only the topographic parameters (tanß, a) are generally calculated, whereas the remaining three hydraulic parameters are normally obtained through calibration.

Topographic parameters

As far as tanß and a are concerned, their calculation has been greatly simplified with the introduction of digital elevation models and the development of digital terrain analysis methods (see Beven and Moore, 1993). But whereas the calculation of local slope is a fairly straightforward procedure, whatever the type of DEM adopted, the calculation of accumulated upslope area poses some problems.

These problems are essentially due to the type of algorithm used to calculate flow paths within the catchment, and the implications this has on the representation of flow processes. Quinn et al. (1995a) carried out a comparison of the single flow path algorithm proposed by O'Callaghan and Mark (1984) and the multiple flow path algorithm, the latter based on the work of Quinn et al. (1991). Their research did not consider a spatially variable T_0, but rather focussed exclusively on the ln(a/tanß) topographic index. Their results indicate that:

a) the multiple flow path approach gives a more realistic pattern of accumulating area on the hillslope portion of the catchment;
b) the single flow path approach is instead more suitable once the flow has entered the more permanent drainage system.

Furthermore, the type of algorithm adopted has been shown to significantly influence the cumulative distribution function of ln(a/tanß) (Fig. 3.5). When the single flow path algorithm is used, the value of tanß is consistently higher due to the fact that the gradient considered is always the steepest, rather than an average of all downslope gradients (Quinn et al., 1991). Consequently the values of the topographic index are, on the average, lower for the single flow path approach. These results have recently been confirmed by research carried out by Wolock and McCabe (1995), where the results obtained with the two flow path algorithms were compared.

Another aspect which has received some attention by researchers regards the separation of hillslope cells from river network cells, which can have a significant effect on the topographic index distribution (Quinn et al., 1995a, Saulnier et al., 1997a). The reason for this is that if river cells are not flagged as such, any flow path algorithm will assign to them the total catchment area drained by the channel.

Consequently, the effect will be a bias towards artificially high index values for the river cells, and this is not consistent with the wetness index concept which is intended to reflect saturation conditions on the hillslopes. Instead, if the river cells are flagged as such, then the upslope drained area can be calculated relative only to the portion of hillslope drained by each river cell. A summary of the various methods, is given by Morris and Heerdegan (1988) and many of them rely on the determination of a Channel Initiation Threshold (CIT) value which has been described in the previous chapter.

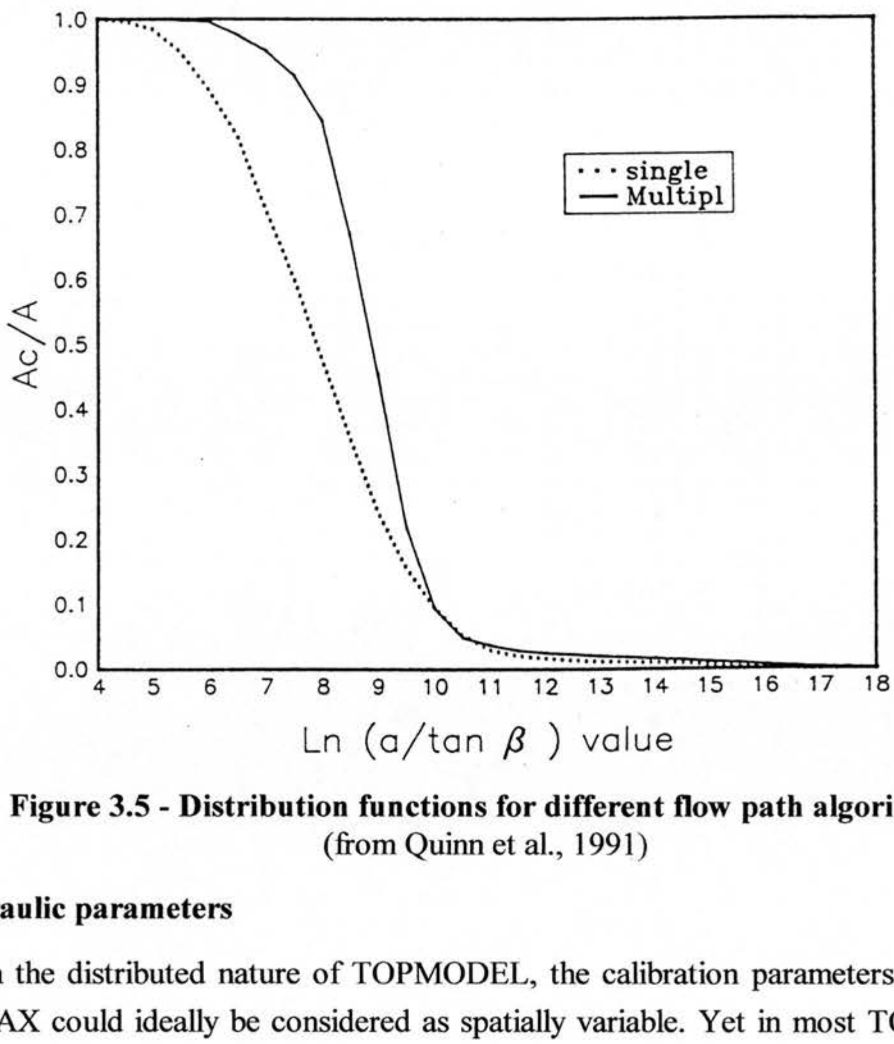

Figure 3.5 - Distribution functions for different flow path algorithms
(from Quinn et al., 1991)

Hydraulic parameters

Given the distributed nature of TOPMODEL, the calibration parameters T_0, m and SRMAX could ideally be considered as spatially variable. Yet in most TOPMODEL applications, the values of T_0, m and SRMAX are generally assumed as constants for the whole catchment (e.g. Quinn and Beven, 1993; Robson et al.; 1993, Wolock and McCabe, 1995). There are different historical reasons for this, and we will briefly examine them for each of the three parameters.

a) The parameter (m) is, as we have already stated, an effective parameter that cannot be directly measured. Furthermore, under the assumption that it reflects the overall behaviour of the catchment storage-transmissivity mechanism, it would not be consistent to distribute it spatially.

b) The maximum root zone storage (SRMAX) is also an effective parameter that summarises the combined interception and evapotranspiration mechanisms. Ideally, if we could characterise both the combined root zone and the interception mechanism to the required degree of spatial resolution, it would be possible to consider a spatially distributed SRMAX. Unfortunately, quantifying the spatial variability of SRMAX would require detailed field measurements to characterise the behaviour of the root zone and interception mechanisms. Even if we could determine SRMAX in a discrete number of points, there would always be the uncertainty inherent in generalising from the measurement points to the pixel scale (Beven, 1989).

c) The lateral saturated soil transmissivity T_0 can be calculated once the saturated soil conductivity (K_0) and m are known (see equation 3.1). Given that the former parameter can be measured as a characteristic soil property it should be possible to spatially distribute T_0. But even where this information is available, this option has generally not been implemented in the past because, as Quinn and Beven (1993), p. 429) point out, a good description of topography is of greater importance

> "due to its much larger variance at the catchment scale and hence the distribution of T_0 will be approximated by its mean value."

The calibrated value of T_0 is therefore often assumed to represent an average transmissivity for the whole catchment (Quinn et al., 1991; Robson et al, 1993; Pinol et al., 1997). This assumption will be verified in relation to the soil classifications used for calculating saturated conductivity and T_0.

3.4 Modular Structure of TOPMODEL

The standard TOPMODEL suite of programs can be applied both to single catchments or to a set of subcatchments comprising a larger catchment. In the latter case, the user can specify different topographic index distributions for each subcatchment and obtain runoff predictions at each subcatchment outflow point. In either case though, the calibration parameters (m, SRMAX, T_0) and the initial flow conditions (Q_{INI}) have in the past been assigned as constants for all subcatchments.

It was initially thought that the multiple subcatchment version of the model could be used to calculate the spatially distributed soil moisture deficit of a chosen subcatchment. Upon closer examination of the code though, it was found that the model structure led to a significant conceptual inconsistency. In particular, the initial timestep of a simulation is always chosen so that the observed flow (Q_{INI}) is assumed equal to the subsurface flow (Q_b), with no saturated excess overland flow. Consequently, from equation (3.11) we can derive the initial average soil moisture deficit for each subcatchment

$$SBAR_i = -m\ [\ln(Q_b/q_o)_i] = -m\ [\ln(Q_{INI}/q_o)_i] \qquad \text{(Eqn. 3.18)}$$

where $q_o = \exp(-\gamma)$ and therefore varies for each subcatchment as a function of the catchment average soil topographic index (γ). But because Q_{INI} is assumed to be constant for all subcatchments, the initial average soil moisture conditions may not reflect the actual observed flow of the individual subcatchments. It is therefore conceptually incorrect to try and predict the soil moisture states of a subcatchment with this version of TOPMODEL.

For the reason outlined above, it was decided not to pursue the option of predicting the soil moisture states of any subcatchments using the multiple catchment version of TOPMODEL. All catchments and subcatchments were therefore modelled as a single unit, using the actual observed initial flow of the catchment.

3.5 Conceptual limits of TOPMODEL theory

We can examine the limits of TOPMODEL with respect to two of the key requirements of hybrid index-based models:

1) the use of a minimum number of physically significant parameters;

2) the ability to test and validate model predictions.

It is useful at this point to recall the initial ideas of Beven and Kirkby:

> "The model parameters are physically based in the sense that they may be determined directly by measurement...." (Beven and Kirkby, 1979, p.43).

As the preceding paragraphs have shown this is not always so, especially for the parameters m, T_0 and SRMAX. Nonetheless, research has highlighted the important role m and T_0 play as physically interpretable scaling factors in the relationship between local soil moisture deficit and catchment average soil moisture deficit (Quinn and Beven, 1993). Therefore, even though m and T_0 cannot be considered as true physical parameters, they can be interpreted as physically significant in the representation of catchment processes. The problem with this type of approach is that effective parameters will allow us to correctly represent the global behaviour of a catchment (rainfall-runoff transformation), but they may not always allow us to predict internal states of a catchment (Grayson et al, 1992b). Also, the difficulty in obtaining spatially distributed values of the model parameters (m, T_0, SRMAX) has traditionally limited TOPMODEL researchers from examining the prediction of spatial patterns of hydrological response.

Another aspect to consider regards the hypothesis of quasi-steady state conditions throughout the catchment. The model assumes steady state conditions are a good approximation of the transient conditions between the precipitation of rainfall and the generation of runoff (Beven, 1986a; Quinn et al., 1991). O'Loughlin (1986, p.796) points out that this condition is satisfied in catchments where "drainage flux, hillslope outflow, and the boundaries of saturation zones are slowly varying quantities." But, as Gallart et al. (1997) point out, in dry catchments where the contributing areas show a high seasonal variation the steady-state assumption is not valid. The steady-state assumption also poses some limitations on the value chosen for the time step, particularly in relation to the spatial resolution adopted. In particular, Beven (1986a) points out that the time step must be short enough to allow the model to simulate the dynamic variable contributing areas within storms, but at the same time long enough to allow transmission of overland flow to the channel bank within one time step. Within the present research we will evaluate the assumption of quasi-steady state conditions with respect to the results obtained with spatially variable soil data.

In order to be able to validate model predictions of internal states of the catchment, TOPMODEL can be modified to predict depths to water table. These could be derived from the soil moisture content, with the following equation:

$$Z_i = S_i / (\varnothing_{eff}) \qquad \text{(Eqn. 3.19)}$$

where (Z_i) is the depth to water table and ($\varnothing_{eff}$) is the effective porosity of the soil. This approach has been considered by Quinn et al. (1998), who concluded that a limiting factor was to be found in the availability of sufficient piezometric data and soil porosity data.

In recent years, much research has been carried out to try and generalise or extend the application and theory of TOPMODEL. In particular, the spatial variability of the three key TOPMODEL parameters (m, SRMAX, T_0) has recently received a certain amount of attention within the TOPMODEL community. Yet none of the results published by Saulnier et al. (1998) or Pinol et al. (1997) seem to provide an evaluation of how such spatial parameters could be used in a more application oriented context, nor have they addressed the issue of how such parameters could be derived from spatial soil datasets for generic catchments. Rather, they have concentrated mainly on a process-related evaluation of the model response to hypothetical spatial variations of the input parameters.

As an alternative to the above approach, the present research will attempt to establish an application-oriented methodology that is also capable of explaining known processes of rainfall-runoff transformation. In this manner, it is hoped that the methodology identified might better reflect the needs of practical catchment modelling applications, rather than purely those of process studies.

3.6 The Choice of Field Data and Experimental Catchments

The choice of the catchment(s) to be used for the simulations was a critical aspect of the research. Once a model had been chosen, it was then necessary to identify one or more catchments for which monitoring networks and field studies had collected all the necessary data. Given the wide range of expertise acquired by the Institute of

Hydrology, both in the UK and world-wide, it was decided to approach them initially and discuss the possible options[5].

The main factors considered in the choice of research catchments are listed below.

a) The limited amount of time[6] and resources available to seek out and acquire the necessary datasets.
b) Availability of spatially distributed catchment hydrological measurements.
c) Availability of surveyed soil and soil hydraulic property datasets.
d) Availability of field scientists and modellers with in-depth understanding of processes in the monitored catchment(s).

On the basis of the above factors, it was decided to use the topographic, hydrological and soils data collected by the Institute of Hydrology for its experimental catchments in Plynlimon, Mid-Wales. (Fig. 3.6). The use of the Balquhidder catchments in Scotland (Fig. 3.7) was ruled out due to the more limited amount of data, and also due to a greater uncertainty regarding the quality control on the hydrological datasets (Price, 1996).

The Plynlimon experimental catchments comprise two upland catchments that are the headwaters of both the Gwy (Wye) and the Hafren (Severn) rivers (Newson, M.D., 1976; Kirby et al., 1991). Meteorological and runoff data has been collected since the late 1960s, with most data collection having been automated since the late 1970s. The data from this latter period had been loaded onto an RDBMS database developed by the Institute of Hydrology using ORACLE (Roberts, 1989). The catchments had also been mapped at the 1:5,000 scale, on the basis of an aerial photo survey commissioned by the Institute of Hydrology from Hunting Surveys.

[5] This involved two separate trips during 1995/96, to the Wallingford Head Office and to the Plynlimon Field Office respectively.
[6] Originally within the timeframe of a three year full-time PhD.

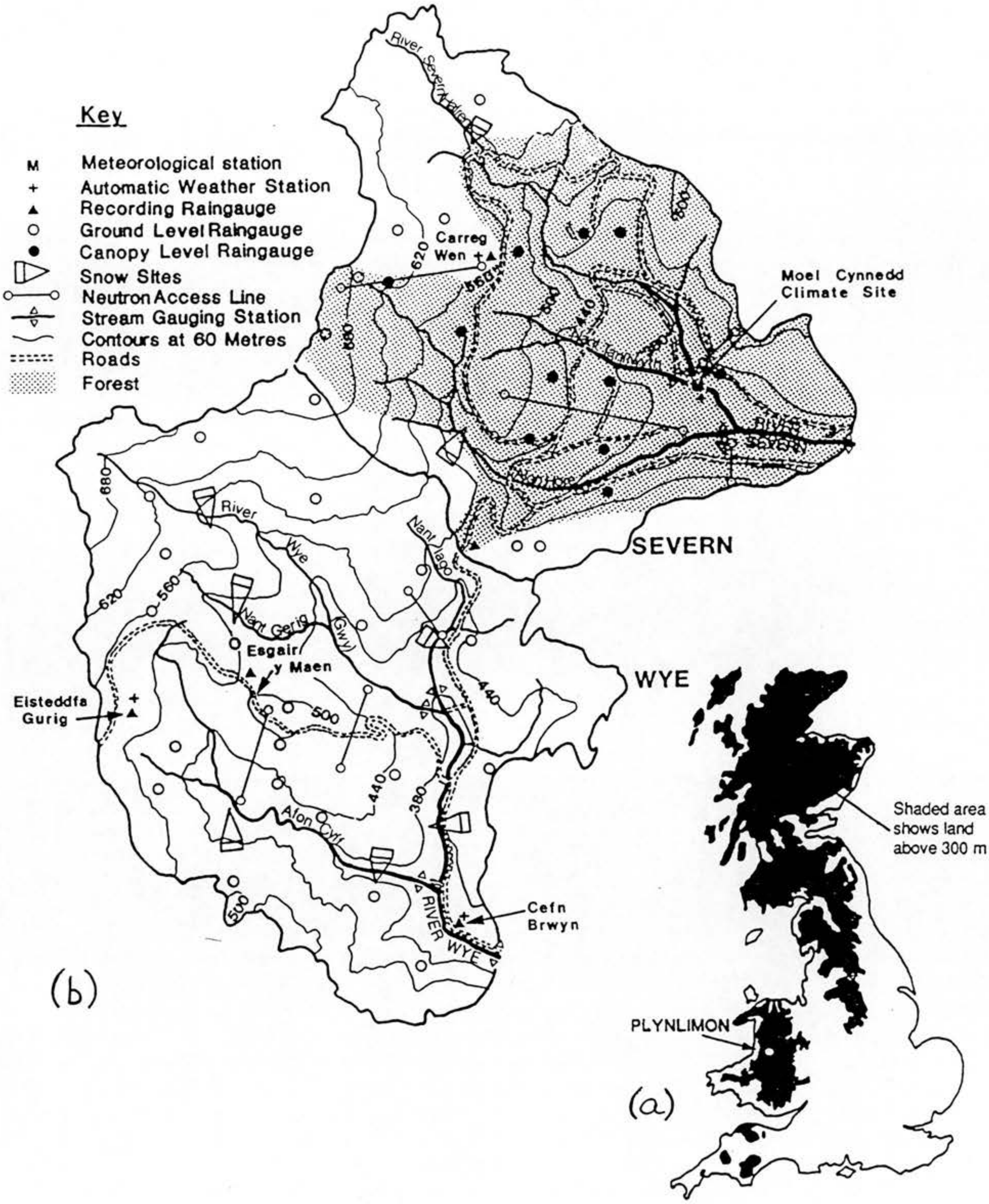

Figure 3.6 - a) Location of the Plynlimon experimental catchments. b) Map of the catchments showing the instrument networks

(from Kirby et al., 1991)

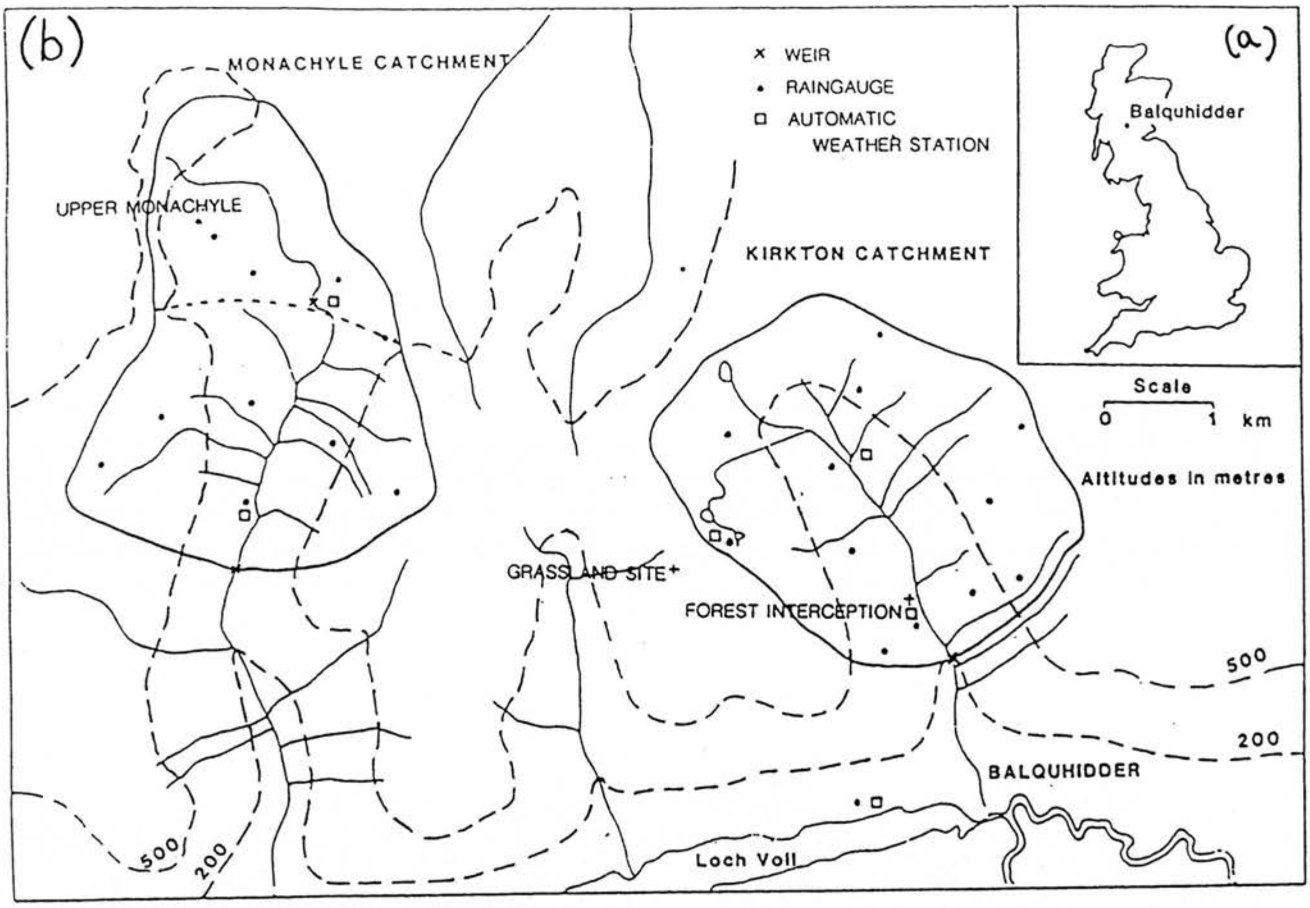

Figure 3.7 - a) Location of the Balquhidder experimental catchments. b) Map of the catchments showing the instrument networks

(from Johnson, 1995)

The catchment monitoring network at Plynlimon has been modified over the years, but the principal elements have included (Newson, 1976)

- hourly rainfall data from tipping bucket continuous recorders;
- monthly groundlevel raingauge data ;
- 15 minute flow data measured for the Gwy and Hafren catchments, as well as for seven of the main tributaries in both catchments;
- hourly Automatic Weather Station (AWS) data including measurements of temperature, net radiation, wind speed, wind direction, used to determine potential evapotranspiration using the Penman-Monteith equations;
- monthly measurements of soil moisture data using neutron probes, located both along hillslope transects and at randomnly positioned sites.

In addition, in recent years a series of 8 piezometer sites in the Hafren catchment had been set up for weekly monitoring of water table levels, with one site also being set up for continuous measurement of water table levels (Neal et al., 1997).

The availability of piezometer data only for the Hafren, together with the subcatchment flow data for the Upper Hore, was considered of critical importance for the spatial validation of TOPMODEL saturated zone predictions. It was therefore decided at an early stage to use only the data from the Hafren for the simulation exercise.

With regard to the choice of a subcatchment for the prediction and validation of internal soil moisture conditions, it was decided to use a headwater catchment where the influence of channel cells would be minimal. Also, given the prevalence of peat soils in upland catchments it was felt important to select a subcatchment that had a high percentage of peat soils and a smaller variability in topography. The latter was an important condition in order to limit the maximum values of the topographic index. This would therefore make the soil-topographic index distribution more sensitive to the influence of a spatially distributed K_0. All of the above reasons, together with the need for measured flow data, led to the choice of the Upper Hore subcatchment, for which the flow measurement structure is shown in Fig. 3.8.

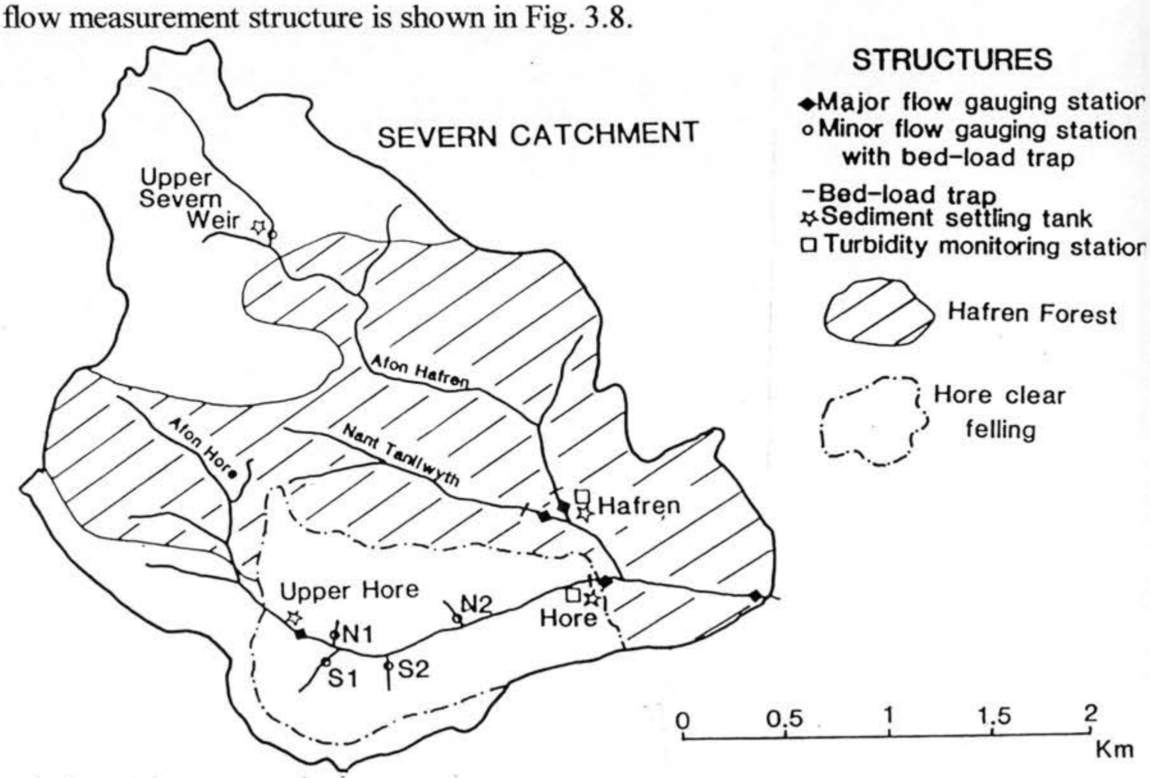

Figure 3.8 - Map of the Measurement Structures in the Hafren

(from Kirby et al., 1991)

3.6.1 Soil Hydraulic Properties

With regards to data on soil properties, the Institute of Hydrology has not carried out extensive field surveys for the measurement of saturated soil transmissivity (Hudson, 1996). Chappell and Ternan (1992) and Soulsby (1992) report on findings relating to measurements of vertical K0 on hillslopes in two different catchments in the Plynlimon area, but their measurements have been concentrated on selected hillslopes and have not included the hilltop or valley-bottom peats and mires.

An examination of the Soil Map of England and Wales 1:250000 (SSOEW, 1983) revealed the presence of only two major soil associations in the Plynlimon area, which were the Crowdy 1 (1013a) and the Hafren (654a). Fortunately, a higher resolution soil map at 1:10000 scale has also been produced by the former Soil Survey of England and Wales (Hartnup, 1988), which details all the major soil series found in the catchments. A summary of the general characteristics of the soil associations, and the associated soil series shown on the map, is given in Tab. 4.1. The complete description of the classification system used is given by Avery (1980) and Clayden and Hollis (1984).

It was initially hoped to apply the methods developed by the Soil Survey and Land Research Centre (SSLRC)[7] for deriving soil hydrologic properties from easily measurable physical properties (bulk density, organic carbon content, sand/silt/clay content, drainable pore space, etc.). This methodology, incorporated into the SEISMIC land information system (Hallett et al., 1995), is based on the pedotransfer functions developed by Van Genuchten (1980) and the empirical saturated conductivity equations derived by (Hollis and Woods, 1989). The advantage of the SSLRC method lay in the possibility of obtaining both vertical and lateral K_0, as well as effective porosity, for all soil types and a wide range of land uses. The latter two parameters were required by TOPMODEL to calculate soil transmissivity and to predict water table depths instead of soil moisture deficit.

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[7] Formerly the Soil Survey of England and Wales.

Soil Code	Soil Association Major soils series	Geology	Soil & Site Characteristics	Cropping & Landuse
311 b	SKIDDAW - Skiddaw - Hiraethog - Winter Hill	Palaeozoic slaty mudstone and siltstone	Very shallow very acid peaty upland soils over rock often on steep slopes. Some deeper peaty-topped soils with ironpan. Thick peat on gentler slopes. Bare rock locally.	Stock rearing on wet moorland habitats of moderate grazing value in the uplands and mountains; recreation.
561 c	ALUN - Aled - Enborne - Trent	River alluvium	Deep stoneless permeable silty soils. Some similar/fine loamy soils variably affected by groundwater. Over gravel in places. Flat land. Risk of flooding.	Dairying and stock rearing on permanent and short term grassland;some cereals where flood risk low.
611 c	MANOD - Manod - Denbigh - Powys	Palaeozoic slate, mudstone and siltstone.	Well drained fine loamy or fine silty soils over rock. Shallow soils in places. Bare rock locally. Steep slopes common.	Stock rearing and woodland in uplands; some dairyin and cereals in Devon and Cornwall with woodland on slopes.
654 a	HAFREN - Hafren - Hiraethog - Wilcocks	Palaeozoic slaty, mudstone and siltstone.	Loamy permeable upland soils over rock with a wet peaty surface horizon and bleached subsurface horizon, often with thin ironpan. Some peat on higher ground. Rock and scree locally.	Moorland and grassland habitats, of moderate grazing value; recreation; coniferous woodland; stock rearing and dairying on improved pasture.
721 d	WILCOCKS 2 - Wilcocks - Winter Hill - Crowdy	Drift from Palaeozoic sandstone, mudstone and shale.	Slowly permeable seasonally waterlogged loamy upland soils with a peaty surface horizon. Some very acid peat soils.	Stock rearing on wet moorland of moderate grazing value and some permanent grassland; coniferous woodland; recreation.
1013 a	CROWDY 1 - Crowdy - Hafren - Wilcocks	Blanket and basin peat	Thick very acid amorphous raw peat soils. Perennially wet. Hagged and eroded in places. Some slowly permeable loamy soils with wet peaty surface horizons.	Wet moorland and wetland habitats of poor and moderate grazing value.

Table 3.1 – General Description of the Plynlimon Soils
(from Soil Survey of England and Wales, 1983)

A summary of the SEISMIC vertical and lateral saturated conductivities is shown in Tab. 4.2, where the conductivities are given – where known – for each of the soil horizons.

Soil	Symbol	Horizon	Depth (cm)	Vert. K0 (m/hr)	Lat. K0 (m/hr)	Lat/Ver K0	Surface Lateral K0	Depth Avgd. Lateral K0	Source
Aled	Aj	A	0-25	0.0611	0.0441	0.721	0.0441	0.0441	SEISMIC
Aled	Aj	C	25-150	NA	NA	NA	-	-	SEISMIC
Crowdy	Cj	O	0-15	NA	0.6021	NA	0.6021	0.6021	Soulsby, 1992
Crowdy	Cj	O1	15-50	NA	0.6021	NA	-	-	Soulsby, 1992
Crowdy	Cj	O2	50-150	NA	0.6021	NA	-	-	Soulsby, 1992
Hafren	HN	O	0-10	0.8340	0.6021	NA	0.6021	0.1320	Soulsby, 1992
Hafren	HN	Eg	10-25	0.0646	0.0470	0.728	-	-	SEISMIC
Hafren	HN	Bpodz	25-55	0.1709	0.1283	0.751	-	-	SEISMIC
Hafren	HN	BC	55-80	0.0988	0.0724	0.733	-	-	SEISMIC
Hafren	HN	C	80-135	0.1134	0.0988	0.871	-	-	SEISMIC
Hafren	HN	R	135-150	NA	NA	NA	-	-	SEISMIC
Manod	Mj	A	0-25	0.0756	0.0555	0.733	0.0555	0.0467	SEISMIC
Manod	Mj	Bpodz	25-60	0.0895	0.0655	0.732	-	-	SEISMIC
Manod	Mj	C	60-130	0.0485	0.0342	0.705	-	-	SEISMIC
Manod	Mj	R	130-150	NA	NA	NA	-	-	SEISMIC
Skiddaw	Skd	O	0-10	NA	0.6021	NA	0.6021	0.6021	Soulsby, 1992
Skiddaw	Skd	R	10-150	NA	NA	NA	-	-	SEISMIC
Wilcock	Wo	O	0-25	1.9660	1.4195	NA	1.4195	0.2484	Soulsby, 1992
Wilcock	Wo	Eg	25-50	0.0521	0.0370	0.711	-	-	SEISMIC
Wilcock	Wo	Bg2	50-75	0.0231	0.0154	0.667	-	-	SEISMIC
Wilcock	Wo	BC	75-150	0.0105	0.0062	0.589	-	-	SEISMIC

Avg. Lat/Ver Ksat ratio from SEISMIC data = 0.722

Note
- Land use for the soils is "forest" (Soulsby, 1992) or "other" (SEISMIC).

Soil Layer Designation
A = Mineral topsoil
O = Peaty topsoil
O1 = Upper peaty subsoil
O2 = Lower peaty subsoil
Eg = Upper mineral topsoil depleted of iron and/or clay and with evidence of seasonal wetness
Bpodz = Mineral subsoil enriched in some combination of humus, iron and aluminum
Bg2 = Lower mineral subsoil with evidence of wetness.
BC = Transitional layer between a mineral subsoil and relatively unweathered substrate
C = Mineral substrate. This may be relatively unweathered 'soft' unconsolidated material, gravel or rock rubble.
R = Relatively unweathered, coherent rock.

Table 4.2 - Summary of Soil Conductivity Data

Unfortunately, closer examination of the method proposed by Hollis and Woods (1989) revealed that the equations are not easily applicable to organic soils, which cover approximately half of the catchment area (Fig. 4.9). This is due to the fact that for peat soils, it is very difficult to obtain representative measurements of drainable pore space given the extreme variability in soil structure. It was therefore necessary to modify the original approach and identify other sources of saturated conductivity values, especially for the organic soils.

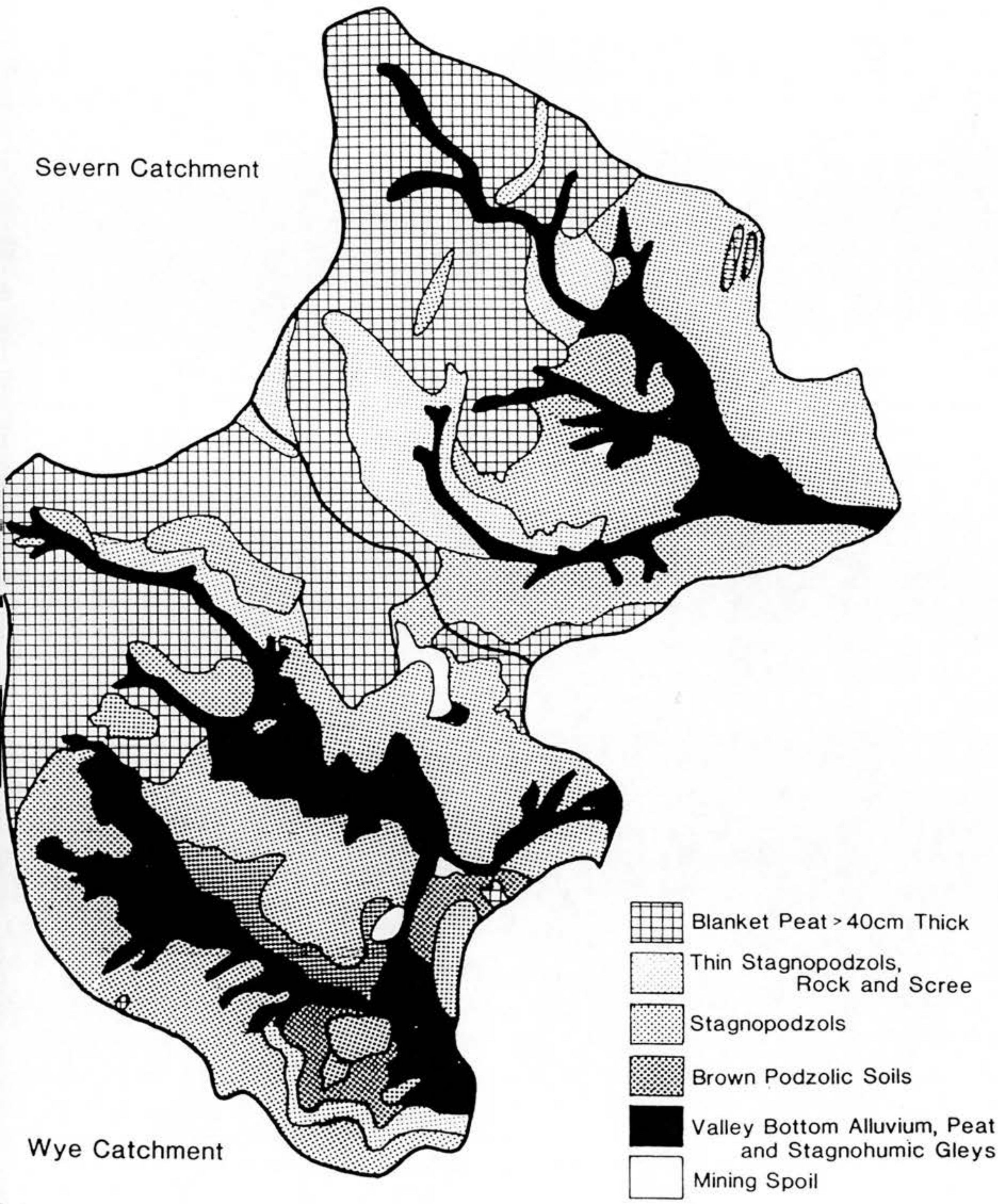

Figure 3.9 - Soil map of the Plynlimon catchments

(from Kirby et al., 1991)

Many studies have been carried out into the measurement of saturated hydraulic conductivities of peats (Stunell and Younger, 1995, Luxmore et al., 1981, Rycroft et al., 1975a). Other studies which have examined the relationship between vertical and lateral K0 (Boulter, 1965, Chason and Siegel, 1986) have found contrasting results. In reviewing the many measurement techniques - both field and laboratory based - of K0 for peats reported in literature, Rycroft et al. (1975b, p. 549) concluded:

> "Evidence in the literature is therefore conflicting and difficult to interpret. It apparently provides an inadequate basis for assessing the relative suitability of the various methods available for measuring hydraulic conductivity of peat."

The above results therefore led to the exclusion of the possibility of carrying out field measurements because:

a) the main objective of the research was to investigate the effect of spatially variable K0 on model performance;
b) it was felt that the issues and problems relating to measurement of K0 in organic soils were very specific to the discipline of soil science;
c) the literature on hydraulic properties of organic soils clearly indicated a high degree of heterogeneity in such soils, both over space and time.

It was therefore decided that attempting to carry out field measurements would not have been justified both in terms of resource and time constraints and, even more importantly, in terms of representativity of measured values.

The only remaining source of data were published values of saturated conductivity (K0) and/or hydromorphic soil classifications from the Plynlimon area. In particular, Soulsby (1992) carried out a series of ring permeater tests in the Llyn Brianne catchment near Plynlimon, though he only considered two of the six soil types present in the area (Tab. 3.2). The K0 values derived from the tests were all vertical conductivities and so before they could be used in TOPMODEL they needed to be converted to lateral conductivities. Given that the SEISMIC data contained both lateral and vertical K0 values for all soils, the average vertical to horizontal K0 ratio - equal to 0.722 - was used as the conversion factor for the Soulsby (1992) vertical K0 values. Also, it should be noted that Soulsby did not carry out any K0 measurements for the peaty horizons of the Crowdy or Skiddaw soils. Given the extreme uncertainty in defining K0 for any peat soils, and the lack of published data, it was therefore decided to assign the Hafren surface lateral K0 value to the peaty "O" horizon of both the Crowdy and the Skiddaw soils.

From the combined dataset of lateral K0 values (Tab. 3.2) two different sets of lateral K0 values were calculated:

a) a surface lateral K0 relative only to the top horizon of each soil type, which will henceforth be referred to as LITT.1;
b) a depth averaged lateral K0 relative to all the horizons of each soil type, which will henceforth be referred to as LITT.2.

The latter case is the more correct if we consider the entire soil profile as transmitting subsurface flow. But in the case of TOPMODEL, the assumption is that saturated transmissivity will decline exponentially with depth and, therefore, lateral saturated flow should occur primarily in the topmost soil layer. This though may lead to excessively high conductivities for the organic soils and for this reason it may also be useful to consider the LITT.2 K0 values. For the subsequent simulations it was therefore decided to use both definitions in order to allow a comparison of results. The above data are summarised, together with other classification schemes in Tab. 3.3

The Wetness Class index is a hydromorphic classification originally defined by the Soil Survey of England and Wales (Rudeforth et al., 1984), particularly for application to lowland agricultural soils. This parameter is a qualitative index that takes into account both soil permeability and climatic conditions. The permeability is estimated on the basis of field assessments of soil texture, structure and packing density, together with laboratory measurements of porosity and K0 data. The climatic factors are used to assign a characteristic duration of zero soil moisture deficit within each calendar year. The combined effect provides a qualitative index which reflects the soil's probability of waterlogging, with the higher classes being those with a lower permeability (or higher groundwater tables) and a longer period of zero soil moisture deficit (see Tab.

3.4). In this sense, the soil Wetness Class index is consistent with the definition of the soil-topographic index in TOPMODEL, and it therefore seemed appropriate to use the Wetness Index as a proxy for saturated hydraulic conductivity.

Soil	Symbol	Hafren Area (m^2)	Upp. Hore Area (m^2)	K0 LITT. 1	K0 LITT. 2	Wetness Class	HOST BFI	HOST SPR
Aled	Aj	17500	-	0.0441	0.0441	1.0	0.80	25
Crowdy	Cj	3887500	915000	0.6021	0.6021	6.0	0.17	60
Hafren	HN	2970000	382500	0.6021	0.1320	5.0	0.38	48
Manod	Mj	47500	-	0.0555	0.0467	1.0	0.60	29
Skiddaw	Skd	995000	332500	0.6021	0.6021	5.0	0.26	60
Wilcock	Wo	740000	-	1.4195	0.2484	5.0	0.24	59
Hafren area weighted average				**0.6678**	**0.4064**	**5.4190**	**0.2620**	**55.5570**
Upp. Hore area weighted average				**0.6021**	**0.4918**	**5.5613**	**0.2376**	**57.1841**

Notes
- LITT.1 is the distribution for near-surface values of K0
- LITT.2 is the distribution for depth-averaged values of K0

Table 3.4 – Soil classifications used and associated saturated conductivities

Wetness Class	Duration of Waterlogging
1	The soil profile is not waterlogged within 70cm depth for more than 30 days[1] in most years[2].
2	The soil profile is waterlogged within 70cm depth for 30-90 days in most years.
3	The soil profile is waterlogged within 70cm depth for 90-180 days in most years.
4	The soil profile is waterlogged within 70cm depth for more than 180 days, but not waterlogged within 40cm depth for more than 180 days in most years.
5	The soil profile is waterlogged within 40cm depth for 180-335 days , and is usually waterlogged within 70cm depth for more than 335 days in most years.
6	The soil profile is waterlogged within 40cm depth for more than 335 days in most years.

Note 1 The number of days specified is not necessarily a continuous period.
Note 2 *In most years* is defined as more than 10 out of 20 years.

Table 3.4 - Soil Wetness Classes

Finally, as a more recent example of hydromorphic classification of soil types, the BFI and SPR indices from the HOST Soil Classification (Boorman et al., 1995) are also provided. Though not physically derived from K0, it has been suggested that the two indices could be used as a statistically-based proxy index for K0 (Boorman, 1996). In that sense, the index values should not be considered as physically representative of actual K0 values but, as with the Wetness Class index, only as a qualitative distribution of spatial variability. The values of SPR and BFI coefficients for the Plynlimon soils are shown in Tab. 3.4.

3.7 Integration with GIS

Given TOPMODEL's need for spatially distributed input data, it lent itself easily to varying degrees of integration with GIS. But in order for the integration to provide the most benefit, it was important to first of all identify the specific requirements of the modelling software with respect to spatial data. In terms of datasets, the minimum requirements were:

1) a Digital Elevation Model (DEM) containing catchment topography;
2) a soil map containing all the soil types found within the catchment.

Before carrying out the actual simulations though, it was necessary to preprocess the DEM in order to:

1) verify and, eventually, eliminate any sinks in the DEM;
2) extract the topographic index distribution curve;
3) extract the soil-topographic index distribution curve.

The above operations clearly entailed the use of spatial algorithms and could have been carried out either within a GIS package, or using programs written specifically for the task.

The review of published examples of integration strongly showed how a complex integrated GIS-modelling environment was not necessarily the most appropriate. In particular, it was felt that given the exploratory nature of the work, a high level integration would not provide the necessary flexibility. Because of the possible need to modify the DEM analysis algorithms based on the results obtained, it was decided to opt for external programs. This option was also facilitated by the fact that the TOPMODEL suite of programmes included auxiliary modules to preprocess the input data. In particular, the *sink.for* programme identifies and fills sinks in the raw DEM file, using an iterative algorithm that identifies the elevation of the lowest neighbour cell in a 3x3 window, adds 0.1m relative to this neighbour and then assigns this value to be the new elevation of the sink. In this manner, the corrected elevation will never be associated to a zero slope value with respect to any neighbour in the 3x3 window. The *gridatb.for* programme then calculates the topographic index distribution for the corrected DEM, based on the multiple flow path algorithm described by Quinn et al. (1991). Finally, the incorporation of spatially variable K0 into the soil-topographic index was not possible within existing programmes and for this reason new code had to be written. This latter aspect will be discussed more fully in section 3.8.

Apart from the specific requirements pertaining to the DEM analysis, there were more important aspects that the integration of TOPMODEL with a GIS had to address. In particular, there were three questions regarding model parameterisation and the output of spatially distributed catchment data.

1) What level of integration was required to allow TOPMODEL to use spatially distributed input data and provide appropriate output of predictions of internal states of catchments?
2) Could GIS help evaluate the effect of uncertainty and error in soil properties, as far as the soils-topographic index [$\ln(a/T_0\tan\beta)$] is concerned?
3) Could GIS be used to identify an appropriate wetness index that would allow TOPMODEL to best represent both the global behaviour and the internal states of catchments?

With regard to the first question, the answer was relatively straightforward. Like many of the low-level integration approaches found in the literature, the present research was interested more in the process-related aspects associated with the use of spatial data than in the actual problems of software integration. Furthermore, given that

a) complex and repetitive data import/export operations were not envisaged,
b) sensitivity analyses in TOPMODEL only considered a limited number of spatial distributions of K_0,
c) graphical map outputs of TOPMODEL results were only necessary for a limited number of simulations, and
d) much of the DEM data preprocessing was possible with already written Fortran programmes,

it seemed a low-level integration would be appropriate and efficient in providing answers to the first question.

In order to consider the effect of uncertainty and error in soil properties data, other soil-related research has relied on significant amounts of field measurements in order for the error analysis to be statistically significant (Heuvelink et al., 1989; Burrough et al., 1992). Initially, it was hoped that the SSLRC - SEISMIC soil data would provide an estimate of variance associated to each soil type. But upon closer examination it was discovered that the variance values had been calculated from a limited number of UK wide samples (Hollis and Woods, 1989). Furthermore, given that the HOST classification did not provide any such measures of variance and that the possibility of field-sampling of data was ruled out, such an approach was not pursued further.

The third question is whether GIS can be used to identify an appropriate definition of wetness index including, among the many possible variables, topographic slope, aspect, soil properties, upslope drained area, etc.. As Western et al. (1999) have highlighted, it is vital that the index is able to account for the dominating physical factors that control the rainfall-runoff transformation mechanism. Therefore, in that respect, the definition of a wetness index cannot rely solely on a complex exercise in spatial analysis and/or geostatistics. Given that the latter are the strengths of a GIS approach, they are of limited use without an adequate understanding of the physical processes. If present trends in research are of any indication, it actually seems that the ability to validate the index with field data is the most important aspect. Consequently, apart from facilitating the calculation of the index from spatially distributed input data, it appears that GIS can contribute little to the identification of appropriate wetness indices.

The last remaining aspect to consider regarded the actual choice of the GIS package to use. The review of published research has shown how the most widespread packages are ARC-INFO and GRASS, both within research institutions and also in the wider context of environmental and hydrological agencies. The principal advantage of GRASS derives from its' historic tradition of a free and very flexible package written in C, for which many users have contributed additional modules specifically for hydrological applications. ARC-INFO on the other hand, is presented as being a complete proprietary package that already contains all of the most requested hydrological functions, as well as full digitising and data editing functionality. Upon closer examination, many users do actually discover that the in-built functionalities may not always be adequate for specific applications. For example, in the particular case of TOPMODEL, ARC-INFO only provides a single-flow path algorithm thus limiting the investigation of other flow-path approaches. Nonetheless, if the user is only interested in a low level integration, both ARC-INFO and GRASS are essentially equivalent. But due to the fact that ARC-INFO was the main package in use at the Dept. of Geography of the University of Edinburgh, and that there was a wide breadth of expertise on which to build, the present research was carried out using ARC-INFO. For the final production of maps ArcView was used instead, given its compatability with ARC-INFO coverages, and the greater ease in preparing quality map plots.

3.8 Modifications to TOPMODEL

Following the examination of the theoretical basis of TOPMODEL, we can conclude that the model satisfies the requirement for a hybrid process-based model that attempts to represent the spatial heterogeneity and temporal dynamics of saturated runoff-generation areas. What remains to be confirmed, is how much the internal state predictions can be improved by introducing spatially variable soil conductivities. In order to allow this evaluation to be performed, the following modifications to the standard code were necessary:

1. the functionality to handle a spatially variable K_0 and calculate the associated soil-topographic index;
2. the option to normalise the spatially distributed K_0 data by a given scaling factor;
3. the calculation of spatially distributed soil moisture deficit data at user-defined timesteps.

The major problem in the standard TOPMODEL code was that the soil transmissivity parameter (T_0) was actually not allowed to vary spatially. The distribution function of the topographic index [ln(a/tanβ)] was calculated from a DEM, by the *gridatb.for* programme, and then T_0 was considered as a constant for the entire catchment.

In particular, the standard TOPMODEL code calculates the T_0 parameter from the soil lateral saturated conductivity (K_0) and the recession parameter (m), through equation (3.1):

$$T_0 = m\,K_0 \qquad \text{(Eqn. 3.1)}$$

and the vast majority of TOPMODEL applications have assumed a spatially constant value of m and K_0, and therefore of T_0. Furthermore, instead of being input as a measured parameter, K_0 has been used as a calibration parameter.

In the modification of the code, the fundamental aspect to consider was that while the (a/tanβ) value is constant for each DEM cell, the value of K_0 would vary according to the different ways of assigning soil properties. Consequently, for every spatial distribution of K_0 we would need to recalculate the spatial distribution of the soils-topographic index. To avoid having to rerun the *gridatb.for* module for every individual K_0 distribution it was decided to modify the main TOPMODEL module so that the soil-topographic index distribution would be calculated at runtime.

The conceptual structure of the modified code is illustrated in the flow-chart in Fig.

3.10. Essentially, the alteration involved adding an IF-THEN loop to allow the user to specify if K_0 is spatially constant or variable. In the former case, the calculation is identical to that in the original code. Starting from the initial ln(a/tanβ) distribution derived from the DEM analysis and given that $\ln(T_0)$ is constant for all cells, we can thus calculate:

$$\ln\left(\frac{a}{T_0 \tan\beta}\right)_i = \ln\left(\frac{a}{\tan\beta}\right)_i - \ln(T_0) \qquad \text{(Eqn. 3.20)}$$

for each index class (i). Consequently, what varies is the index value associated to each class, and not the number of cells in each class.

In the presence of spatially variable K_0, it is not possible to use the already calculated distribution of ln(a/tanβ). Instead, we must calculate the soils-topographic index for each cell in the catchment:

$$\ln\left(\frac{a}{T_0 \tan\beta}\right)_{x,y} = \left[\ln\left(\frac{a}{\tan\beta}\right) - \ln(T_0)\right]_{x,y} \qquad \text{(Eqn. 3.21)}$$

and then consequently sort the cells into a discrete number of index classes. This lengthens the run-time of the program, especially for high resolution DEMs.

The code has also been modified to allow the user to correct the spatially variable K0 values so that their spatial average is equal to a predefined constant. The justification for this is that once an initial lumped calibration is carried out for the catchment, a spatially averaged value of K_0 can be defined. We can then choose to normalise the spatially variable values of K_0 so that their spatial average coincides with the calibrated value. This essentially allows the user to examine the effect of different spatial values of K_0 on the representation of internal catchment processes (eg. soil moisture deficit), without modifying the overall catchment behaviour.

Finally, an auxiliary module was written to allow the model to output the soil moisture deficit (SMD) values for all the catchment cells for any chosen timestep. These values are not normally calculated when the desired output is the catchment outflow. But given the aim of internal validation of model predictions, the modification was carried out to allow the user to obtain SMD maps for the selected timestep. The programme is outlined in the flow-chart in Fig. 3.11.

A detailed listing of the modifications implemented in the code, and described in the paragraphs above, is provided in Appendix 1.

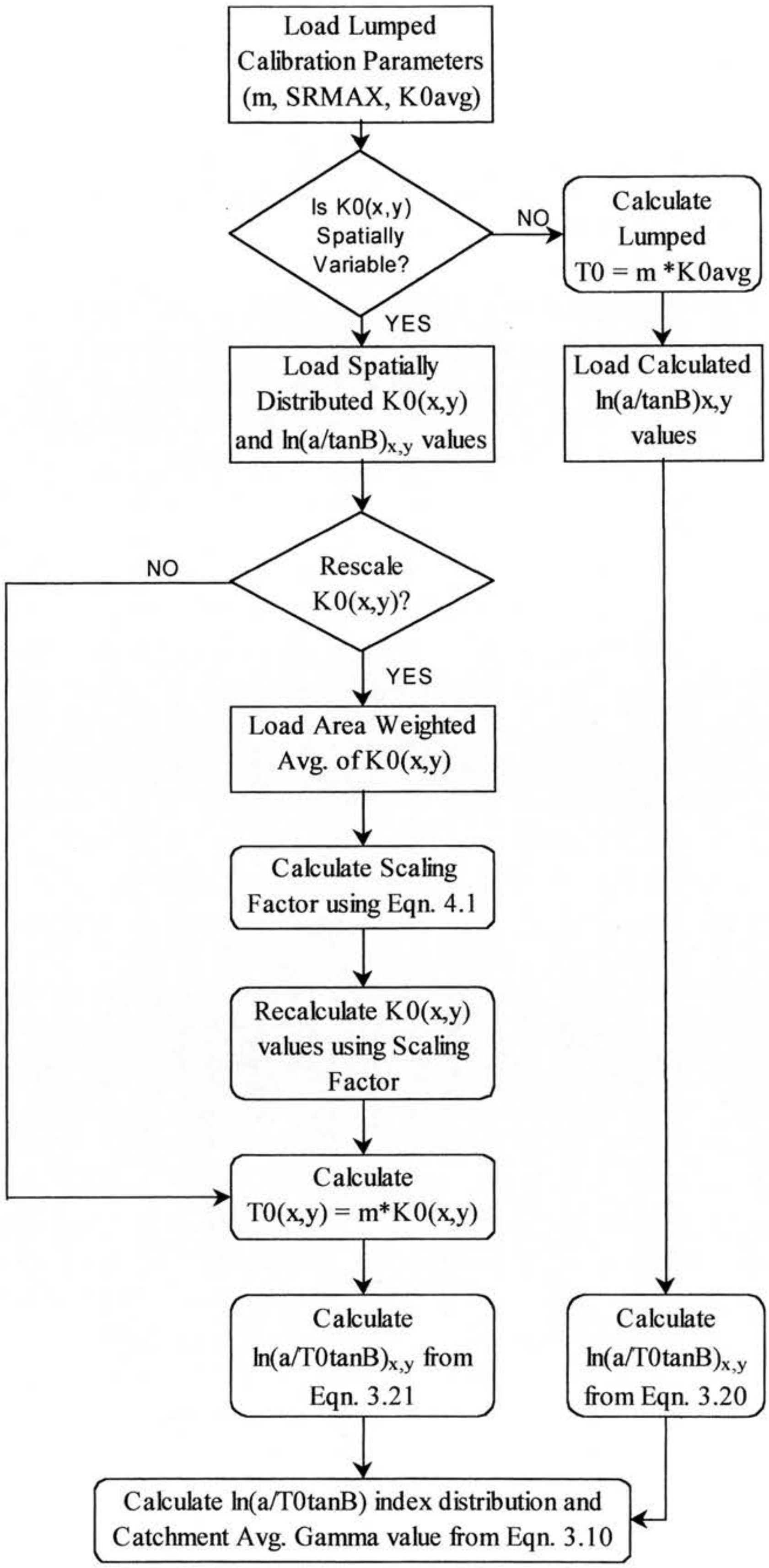

Figure 3.10 - Modified Soil-Topographic Index Calculation

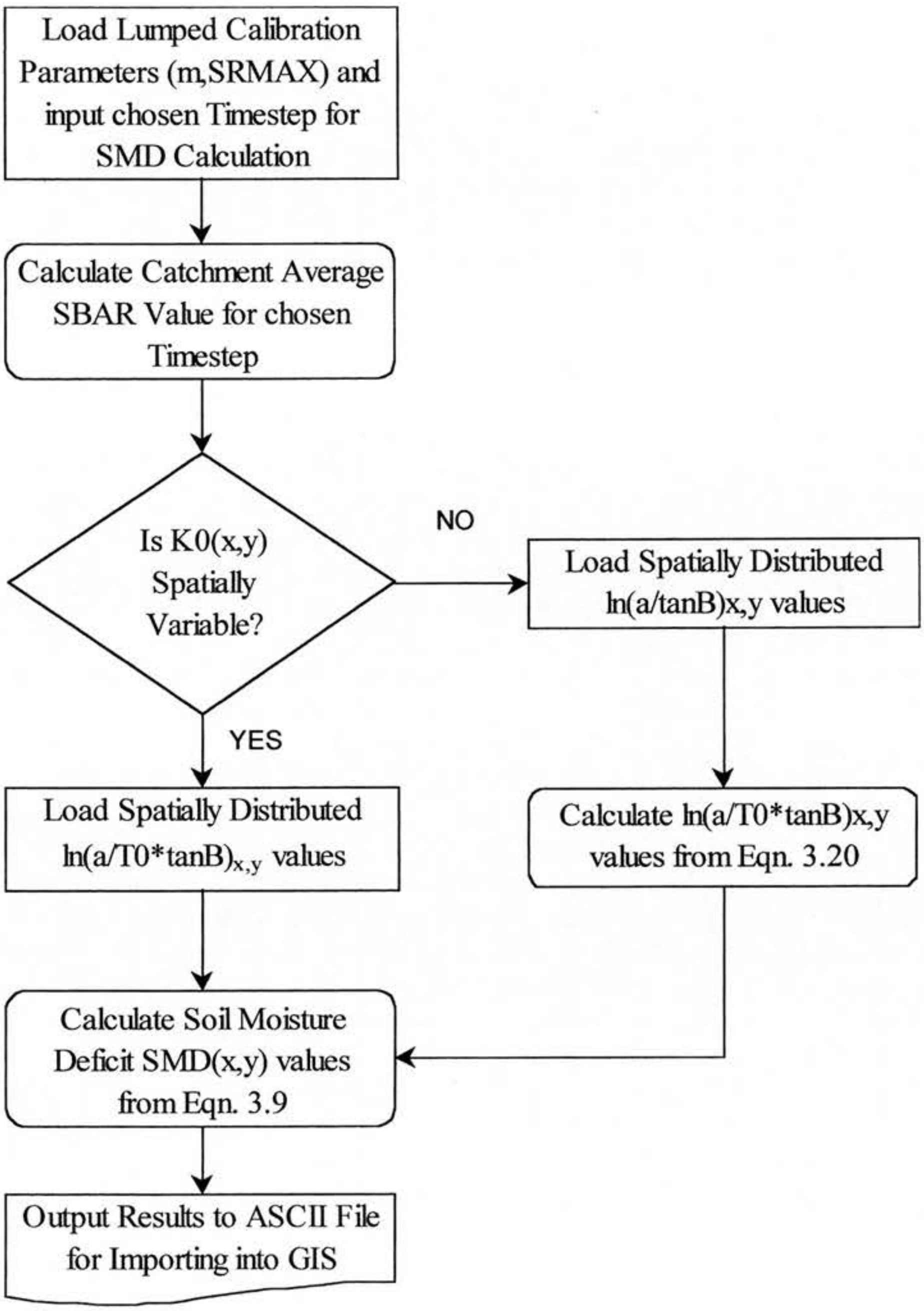

Figure 3.11 - Calculation of Spatially Distributed SMD

3.9 The Modelling Procedure

The initial research approach had envisaged evaluating TOPMODEL performance in the presence of both constant and spatially variable K_0. By validating against internal state variables (water table depth or soil moisture deficit), the method would have both given an indication of model performance and also of the effect of distributed K_0. Clearly, the unavailability of measured K_0 and effective porosity values for organic soils required a verification of the research methodology.

The conclusion reached was that the initial research objective could still be attained if the simulations made use of K_0 distributions derived from literature to investigate how the spatial distributions of K_0 affected TOPMODEL performance. Furthermore, it was decided to also evaluate more qualitative soil classifications (e.g. HOST, Wetness Class) which attempt to express a soil's likelihood to produce runoff. In particular, it was felt that the application of the HOST classification – which had been devised specifically for hydrological modelling – would be a useful exercise with regards to possible "real-world" applications of the proposed methodology.

With regard to the validation of internal states within the catchment, it was decided to simply calculate the soil moisture deficits rather than the water table depths. Unfortunately, the lack of any field measured SMD data meant that the validation would have to be qualitative rather than quantitative. By considering different spatio-temporal scales, it was hoped to be able to identify any scale dependency between soil variability and model performance. The results would allow us to evaluate the sensitivity of TOPMODEL to the spatial distribution of soil saturated conductivities and its' ability to predict saturated runoff generating areas.

The actual modelling phases are described below, and summarised in the flow chart in Fig. 5.12.

1) Carry out preliminary simulations using published values of spatially lumped parameters (m, SRMAX, K_0avg). This was intended to provide an initial appreciation of how TOPMODEL responds to different parameter values.

2) Assuming a spatially lumped K_0, an optimum parameter set of the three calibration parameters (m, K_0avg, SRMAX) was identified. The reason for this was that it was felt that a better performance of TOPMODEL in terms of catchment outflow would also be associated with a more accurate prediction of distributed soil moisture deficit. The evaluation was carried out for different rainfall years, thus providing a parameter set with the best overall behaviour. This set was then used to represent the base case against which all results with spatially distributed K_0 could be compared.
3) With the chosen m and SRMAX parameters, model efficiencies were recalculated using the published LITT.1 and LITT.2 K_0 distributions. This allowed us to evaluate how TOPMODEL behaved using the raw K_0 data.
4) In reality we did not expect the published K_0 data to give valid results because the K_0avg identified in Case 1) is an effective parameter that may not actually be physically representative. In order to obtain more meaningful predictions, model simulations were carried out using normalised values of K_0 scaled so as to make their spatial average equal to the lumped calibrated value K_0avg of Case 1). This phase led to the selection of an optimal soil distribution for the chosen rainfall year, which was also validated on successive years.
5) The input values of K_0 were normalised so as to make their spatial average equal to the lumped calibrated value K_0avg.
6) The model parameters (m, SRMAX, K_0avg) were once again re-optimised for the chosen soil distribution, to verify whether the optimal parameters were influenced by the spatially variable K_0. A final parameter set was therefore selected.
7) To verify the effect of including drainage network cells on the soil-topographic index distribution function, a sensitivity to the Channel Initiation Threshold (CIT) parameter was carried out.
8) Having identified characteristic flood events during a single rainfall year, model efficiencies were calculated using the normalised values of K_0.
9) For the flood events selected in 7) the spatio-temporal patterns of soil moisture deficit were calculated. This was intended to highlight any spatial dependency between soil variability and model performance.

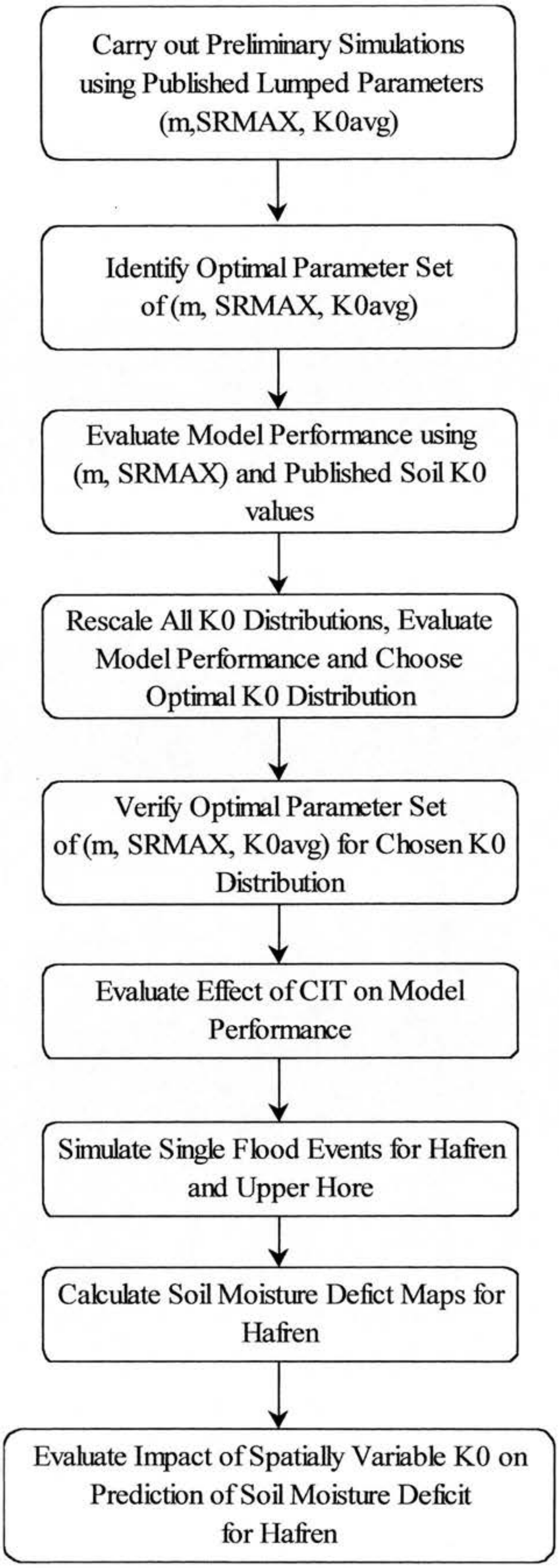

Figure 3.12 - Description of Modelling Procedure

On the basis of the results obtained in the above phases, an interpretation of the results and an evaluation of TOPMODEL's performance was carried out

3.10 TOPMODEL Performance and Validation

The issue of model performance and validation was very important because the simulation procedure described would produce both an integrated catchment response - in the form of catchment outflow - and spatially distributed soil moisture deficit predictions. The initial model validation was carried out on catchment outflows to verify the validity of the spatially lumped calibration parameters. But only by evaluating the performance of the model in terms of soil moisture deficit predictions could we understand the effects of a spatially variable K_0.

With regard to model performance, TOPMODEL uses the efficiency criterion previously discussed in Section 3.3.7 and based on the following equation:

$$eff(\%) = \left\{ 1 - \frac{\sum_{TINI}^{TEND} \left[(Q_{obs}) - (Q_{sim}) \right]_t^2}{\sum_{TINI}^{TEND} \left[(Q_{obs}) - (Q_{avg}) \right]_t^2} \right\} * 100 \qquad \text{(Eqn. 3.22)}$$

Because the efficiency criterion uses all the simulated and observed flow values, it is more sensitive to the temporal variations than methods which rely solely on the comparison of total outflow volumes. Compared to the more commonly used correlation based performance indicators, which use the correlation coefficient (r), Legates and McCabe (1999) state that the efficiency criterion gives a more accurate evaluation of model performance.

Clearly though, the efficiency parameter is still only able to quantify model behaviour with respect to the catchment outflows, and gives no information on how well the model is simulating the spatial characteristics of runoff generation. Another drawback of this method is that the efficiency value is dependent on the variance of the observed flow record. As a result, efficiency values from catchments with radically different flow variances may not be comparable. But in our specific case, it is expected that the variances of the observed flows of the Hafren and Upper Hore will be similar, thus making the efficiency values comparable.

In terms of model validation, different possible approaches will be considered. The simplest and most widely used approach is known as the "split sample test" (Klemes, 1986) and essentially involves:

a) calibrating the model on catchment hydrological data from a specified time period;
b) validating model predicitions on another period in time, as long as we can assume a condition of stationarity for the physical processes being modelled.

This approach is of use particularly when modelling total outflow from a catchment, and indicates how well model calibration is able to represent total catchment behaviour over time. Quinn and Beven (1993) have already applied this approach to the Gwy and Hafren catchments[8] considering a spatially lumped K_0. Their results showed minor variations in model efficiency, thus indicating that TOPMODEL was transposable within similar catchments and over several years.

However, if we intend to evaluate the behaviour of a model in predicting internal states of a catchment, then the validation exercise becomes more complicated. Some possible approaches are listed below.

a) Having identified the best K_0 distribution for a given year, validate the overall model efficiency - based on catchment outflow - for successive years. This will indicate whether the optimal K_0 distribution is constant over time and, if not, this would indicate that some other factor is introducing variability over time.
b) Analyse, for selected flood events, the temporal variations in SMD patterns from the whole Hafren and interpret such variations in terms of observed and predicted catchment behaviour.
c) Compare, for selected flood events, the SMD maps for constant and variable K_0. This would highlight any significant spatial differences between the two distributions, and indicate for which soils the differences are more noticeable.

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[8] Klemes (1986) termed this type of cross-validation for catchments within a region a "proxy-basin" test.

This type of validation would clearly be highly qualitative in nature, especially given that no field measurements of saturation are available. But it is nonetheless hoped that the analysis and interpretation of saturation patterns will still provide useful information to assess the behaviour of the model and the effect of the spatially distributed soil data. More importantly, this approach would evaluate whether "simple spatial modelling combined with qualitative reasoning" (Grayson et al., 1993, p. 83) can actually lead to a greater understanding of model results.

3.11 Conclusions

In the terms outlined in the preceding paragraphs, the primary research objective was to evaluate TOPMODEL performance with respect to spatial patterns of saturation in upland catchments, while using easily available soil conductivity data. The original intention had been to use field-based K_0 values, but this approach had to be abandoned when it was discovered that no data were available for organic/peat soils. Given the need to evaluate alternative sources of published data, the research problem shifted from a more process-based approach to a more application-oriented approach. The methodology described would, through the examination of the effect of spatially variable K_0 data on simulation of distributed rainfall-runoff transformation processes, also allow a critical evaluation of TOPMODEL. In particular, it is hoped that the methodology will provide guidance on the limits of including spatially variable soil data within TOPMODEL and, more generally, within index-based hybrid models.

Furthermore, by evaluating a variety of soil classification systems, the present research hopes to provide some insight into the usefulness of such classifications as input to an index-based hybrid model. Indeed, this type of problem may actually be closer to the interests of the wider hydrological community, where the simulation of ungauged and unmeasured catchments is still a common problem.

Finally, within the limits of a low-level integration with a GIS, the methodology illustrated in this chapter would also attempt to provide a further insight into the limits and advantages of integrating GIS with a spatially distributed hybrid model.

4. Simulation Results

The present chapter describes the results obtained for the various phases of the modelling procedure described in the previous chapter (Section 3.9). It begins by describing the preparation and preprocessing of the hydrological, soils and topographic input data. This is followed by a discussion of TOPMODEL performance for some preliminary parameter sets. The effect of a spatially variable saturated conductivity on model performance is then described, for both full year and single event simulations. Finally, the chapter will close with the results of the spatially distributed soil moisture deficit (SMD) predictions. A brief discussion of all the results will be presented in the present chapter, while a more in-depth analysis, also in relation to the wider research context, will be presented in the following chapter.

4.1 Preparation of Input Data

Having decided on a low-level integration between the GIS and TOPMODEL, the initial role of the GIS was limited to the preparation of the topographical and soil input data. Unfortunately the two packages used different data formats for storing (x,y,z) data and, consequently, two conversion programs - *grid_exp.for* and *grid_imp.for* - were written to automatically convert the data between the two packages. The printouts of the relevant programs are included in Appendix 1. Given the limited number of times that such operations were carried out, the procedure did not prove too laborious and more sophisticated interfaces were not required. Furthermore, given that the hydrological data were provided in ASCII text format, an SQL interface to the Institute of Hydrology RDBMS was not necessary. Nonetheless, the existing programmes could easily be incorporated within an interface to the RDBMS.

4.1.1 Base Maps

The first step in preparing the input data for the modelling exercise was to digitise the topographic and soil maps. The digitisation was carried out using ARC-INFO and the digitised coverages were then pre-processed as described below.

a) Topography (Hunting Survey 1:10000 base map)

- Hafren catchment boundaries and principal blue-line drainage networks were digitised in ARC-INFO (Fig. 4.1a).
- All contours (10m intervals) were digitised in ARC-INFO (Fig. 4.1a).
- All spot heights were digitised in ARC-INFO.
- Contour data and spot height data coverages were combined into a point coverage, in ARC-INFO, containing 25,222 points.
- Interpolation was carried out using the ARC-INFO - IDW function (inverse distance weighting), obtaining DEM grid coverages at 10m, 25m and 50m resolution. The IDW function was chosen because it was indicated (Watson & Philip, 1985) as giving best results for densely sampled points with respect to the variation being sampled. Based on the total number of digitised points, the average sampling density was calculated as 0.3, 1.8 and 7.3 points per cell, for the 10m, 25m and 50m DEMs respectively. This implied that the IDW method was the most suited only for calculating the 50m DEM.
- In fact the 10m and 25m DTM presented a very high number of sinks both inside and on the boundary of the catchment. Even after applying the sink-filling algorithms in GRID and *sink.for* many sinks still remained and could only have been removed by manual correction. The TOPMODEL simulations were therefore carried out using only the 50m DEM, which is shown in Fig. 4.1b.
- The Upper Hore subcatchment boundary was derived from the sinkfree DEM using the GRID WATERSHED function.
- The ARC-INFO grid coverages were converted to ASCII format for use in TOPMODEL. In the conversion process the National Grid coordinates are lost, and all the catchment cells are therefore referenced by row and column numbers.

b) Soils (Hartnup 1:10,000 base map)

- The soil map was registered to the topographic map to ensure coordinate correspondence.
- All soil polygons falling within the Hafren catchment were digitised in ARC-INFO (Fig. 4.2a).
- The polygon coverage was converted to a grid coverage at 50m cell resolution, which is shown in (Fig. 4.2b).
- ARC-INFO soil grids were converted to ASCII format for use in TOPMODEL.
- A summary of the various soil saturated conductivity values for each soil classification is shown in Tab. 4.1. To create the spatial K_0 input files separate look-up tables were used to link each grid cell with a value of K_0. In reading the table, it should be remembered that the two classifications based on published results (LITT.1 & LITT.2) show measured values, whereas the last three classifications provide indices which are used as proxies for K_0. For each of the distributions used, an area weighted average was also calculated and is shown in the table. The area values given for each soil type represent the total surface area of the Hafren and Upper Hore catchments.

Soil	Symbol	Hafren Area (m^2)	Upp. Hore Area (m^2)	K0 LITT. 1	K0 LITT. 2	Wetness Class	HOST BFI	HOST SPR
Aled	Aj	17500	-	0.0441	0.0441	1.0	0.80	25
Crowdy	Cj	3887500	915000	0.6021	0.6021	6.0	0.17	60
Hafren	HN	2970000	382500	0.6021	0.1320	5.0	0.38	48
Manod	Mj	47500	-	0.0555	0.0467	1.0	0.60	29
Skiddaw	Skd	995000	332500	0.6021	0.6021	5.0	0.26	60
Wilcock	Wo	740000	-	1.4195	0.2484	5.0	0.24	59
Hafren area weighted average				**0.6678**	**0.4064**	**5.4190**	**0.2620**	**55.5570**
Upp. Hore area weighted average				**0.6021**	**0.4918**	**5.5613**	**0.2376**	**57.1841**

Notes
- LITT.1 is the distribution for near-surface values of K0
- LITT.2 is the distribution for depth-averaged values of K0

Table 4.1 - Summary of K_0 Spatial Distributions

- From the above table we can see that the peat soils (Crowdy, Hafren, Skiddaw and Wilcock) are characterised by large HOST SPR Index values, which correspond to a higher likelihood of surface saturation while, for the same soils, the HOST BFI index values are small. It is therefore apparent that the two indices show a very different behaviour. Given that the model simulations will focus on runoff generating processes it would therefore appear that the SPR index is the more appropriate one to use. We shall return to this aspect later on in the present chapter.

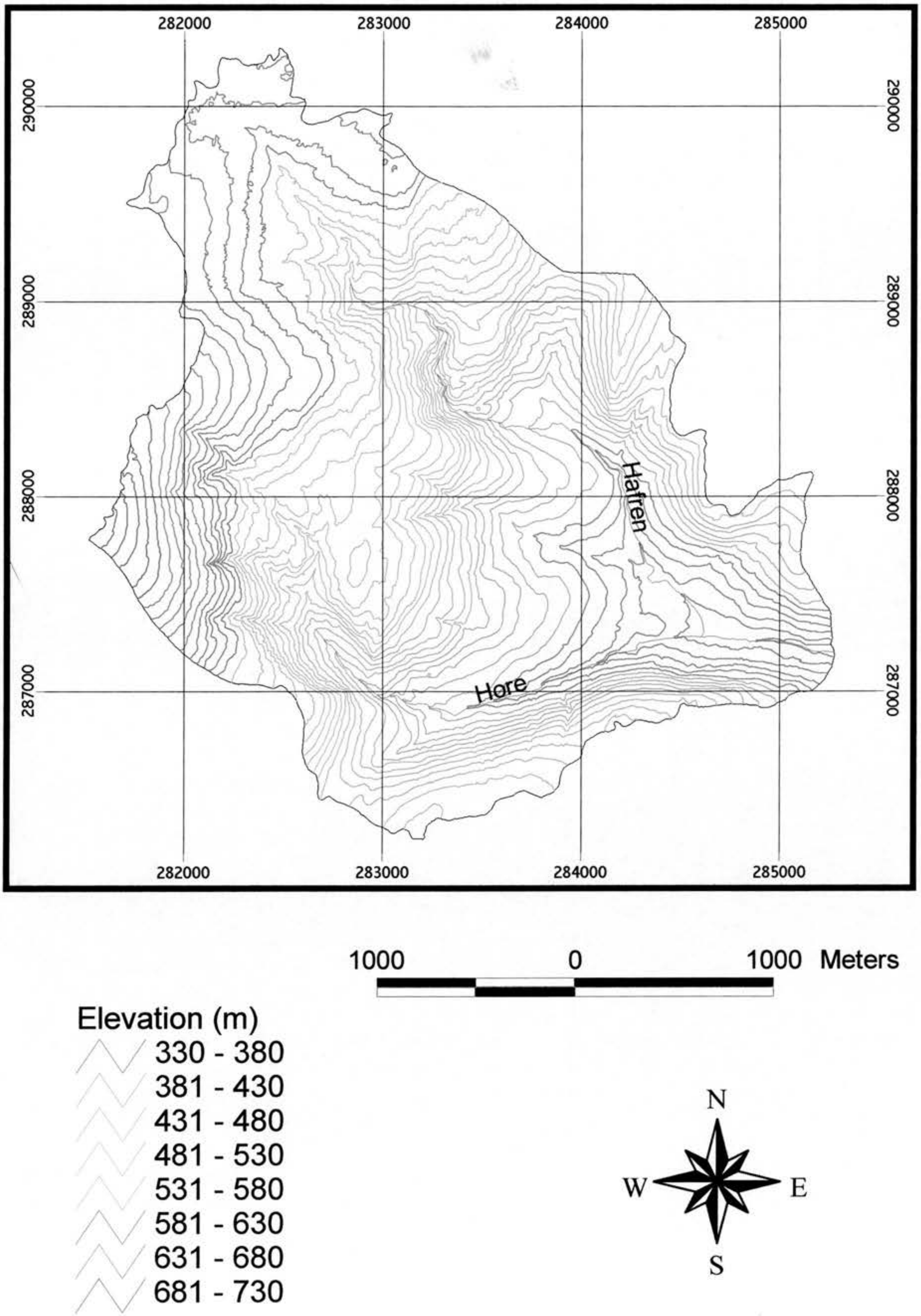


Figure 4.1a - Hafren Digitised Contours

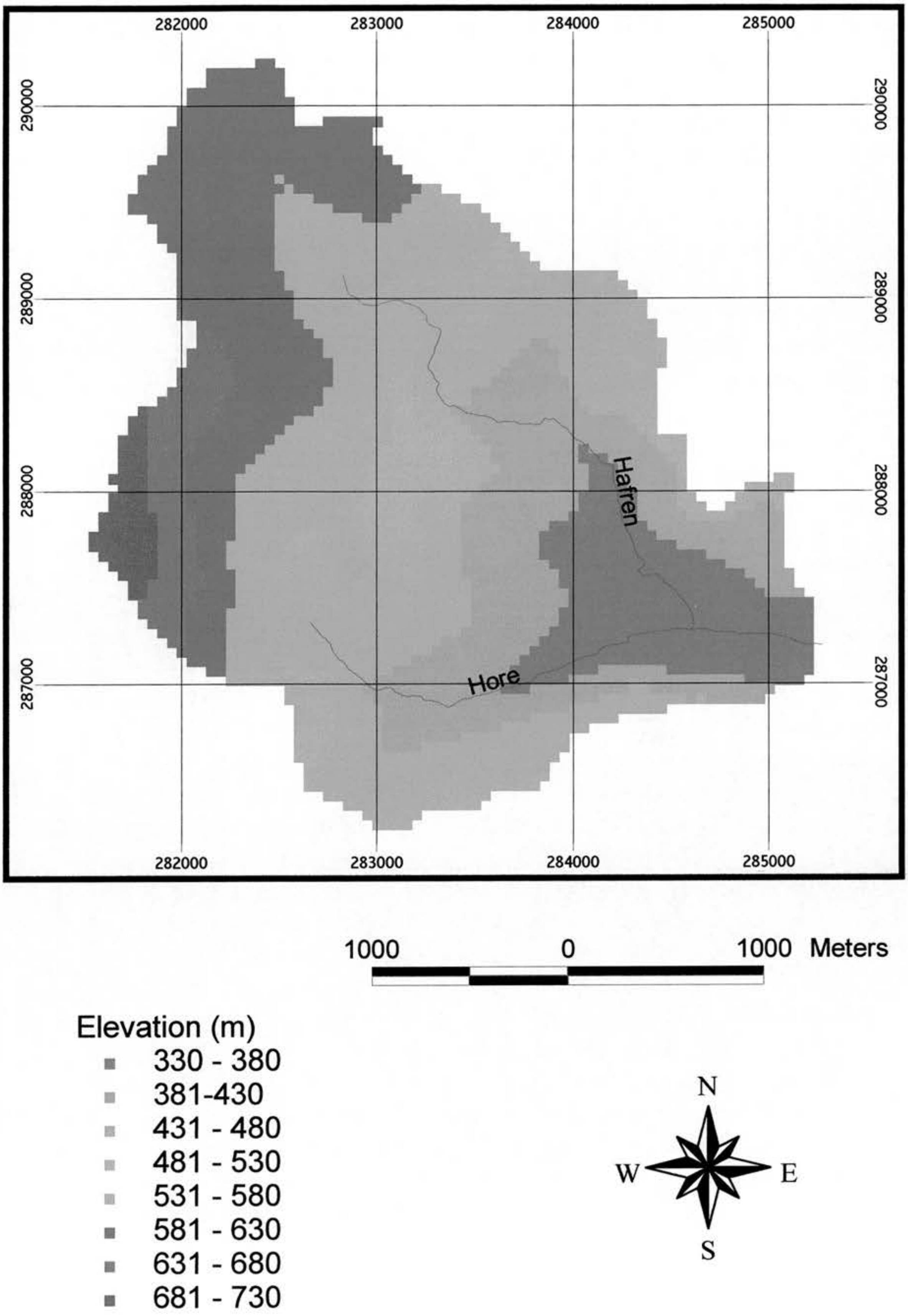


Figure 4.1b - Hafren 50m DEM

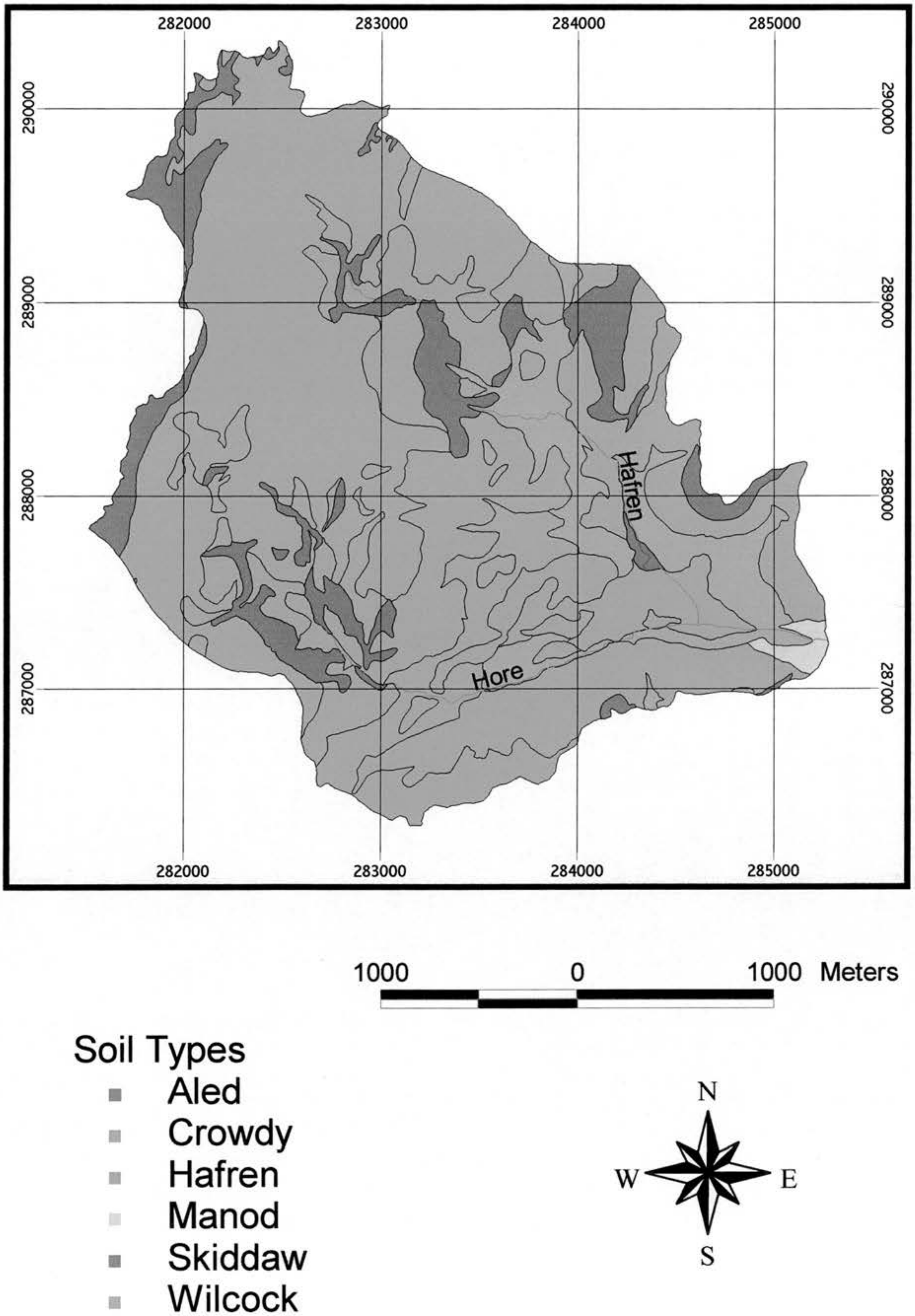


Figure 4.2a - Hafren Digitised Soil Map

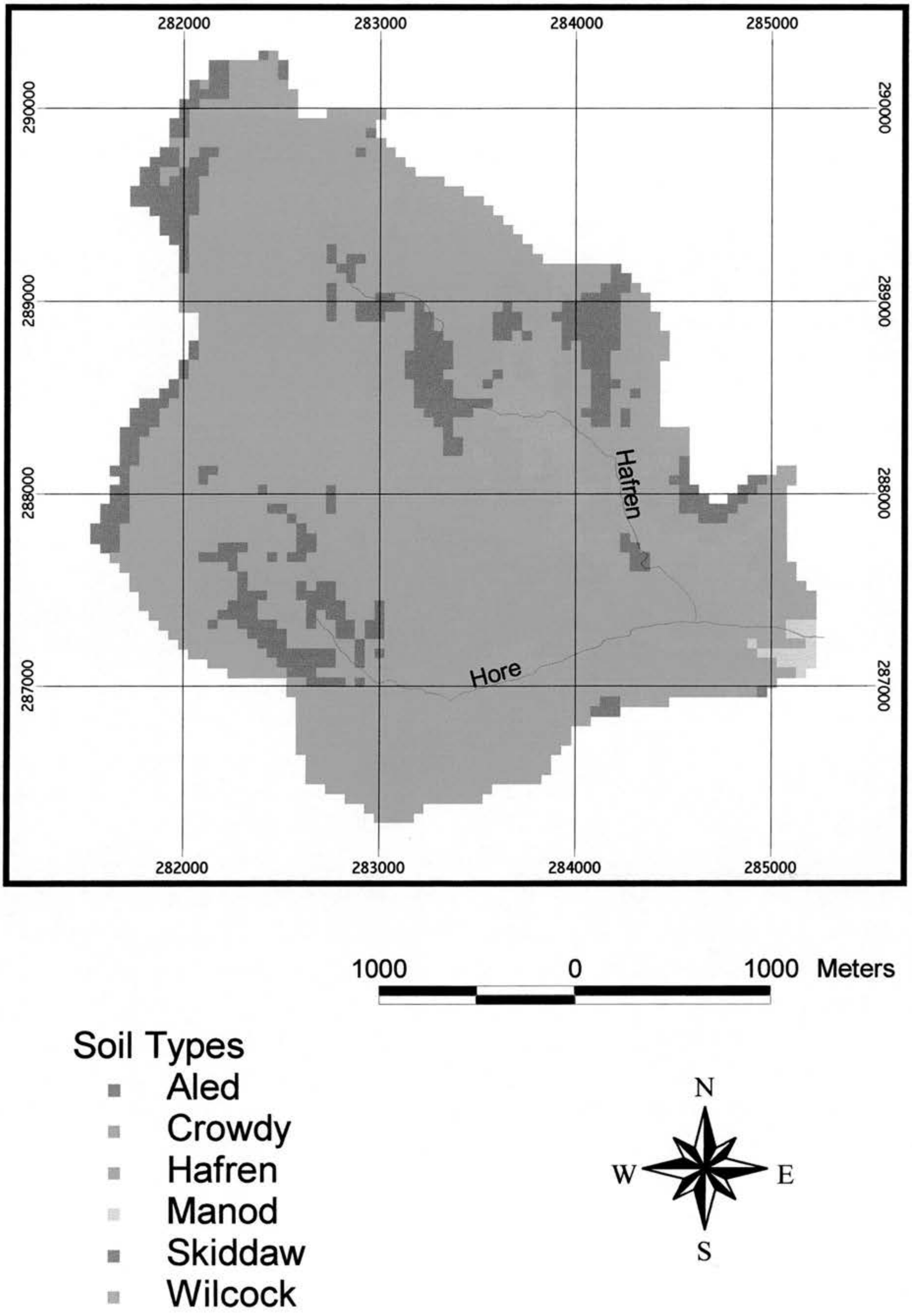


Figure 4.2b - Hafren 50m Soil Grid

4.1.2 Hydrological Data

The necessary files were provided by the Institute of Hydrology (IH) Plynlimon office in ASCII format, ready to be used in TOPMODEL. The specific files provided for the years 1984, 1985, 1986 are listed below. It should be kept in mind that all hydrological data are expressed as volume per unit area, and are therefore shown in metres.

- Spatially averaged precipitation for the Hafren catchment, at 1 hour intervals. It should be underlined that the spatially averaged data was calculated by the Institute of Hydrology as a result of their research on determining mean areal precipitation from the installed raingauge network (Kirby et al., 1991). Unfortunately though this work had only been carried out for the two main catchments, the Hafren and the Gwy. Consequently, this research assumed that the precipitation per unit area values used for the Upper Hore were identical to those of the Hafren.
- Flow data for the Hafren and the Upper Hore measurement gauges, at hourly intervals. For the Upper Hore the Institute of Hydrology only provided data for the year 1985.
- Daily Penman potential evapotranspiration data for the Hafren. Given the lack of more precise data, it was also assumed that the potential evapotranspiration values for the Upper Hore were identical to those of the Hafren.

The rain and flow data for the Hafren 1984-86 and the Upper Hore 1985 data are shown in Figs. 4.3, 4.4 and 4.5. It should be noted that both the rainfall and flow data are always provided per unit area, and are therefore expressed in units of metres/hour throughout the following sections.

In the expectation of validating the TOPMODEL simulations against measured water table data for 1995, the above hydrological data were also obtained for that year.

Unfortunately, due to organisational difficulties within the IH Plynlimon office[1] the water table data for 1995 were never provided. In any case, the unavailability of measured soil hydraulic properties would have required the use of calibrated - rather than predicted - values of effective porosity within the water table version of TOPMODEL. This would have added a further calibration parameter, thus defeating the intent of evaluating field measured variables. This reason provided further justification for validating against spatial SMD predictions rather than spatially distributed water table depths.

Given the presence of snow cover in the Plynlimon area during the winter months, the TOPMODEL simulations had to be carried out only on snow-free months. Based on the Met Office snow data collected by the Institute of Hydrology - Plynlimon, as well as a visual examination of the stored Hafren flow data, the selected simulation periods[2] are summarised in Tab. 4.2. The "Start" and "End" hour columns for each simulation period show the total hours since the beginning of the calendar year.

Years	Start (hrs)	Start (date)	End (hrs)	End (date)	Hafren Initial Obs. Flow (m/h)	Upper Hore Initial Obs. Flow (m/h)
1984	2376	8/4/84	8346	12/12/84	0.00003876	N/A
1985	2496	14/4/85	7896	25/11/85	0.00031912	0.00030425
1986	2376	9/4/86	8472	19/12/86	0.00009124	N/A

Table 4.2 - Snow-free periods for TOPMODEL simulations

[1] The Plynlimon field station closed down in 1999, with responsibility for running the hydrometry networks passing to the Institute of Terrestrial Ecology - Bangor and overall research co-ordination passing to IH - Wallingford (Robinson and Hudson, 1999).

[2] In the remainder of the thesis, I will refer indifferently to simulation periods and simulation years, intending in all cases the snow-free months summarised above.

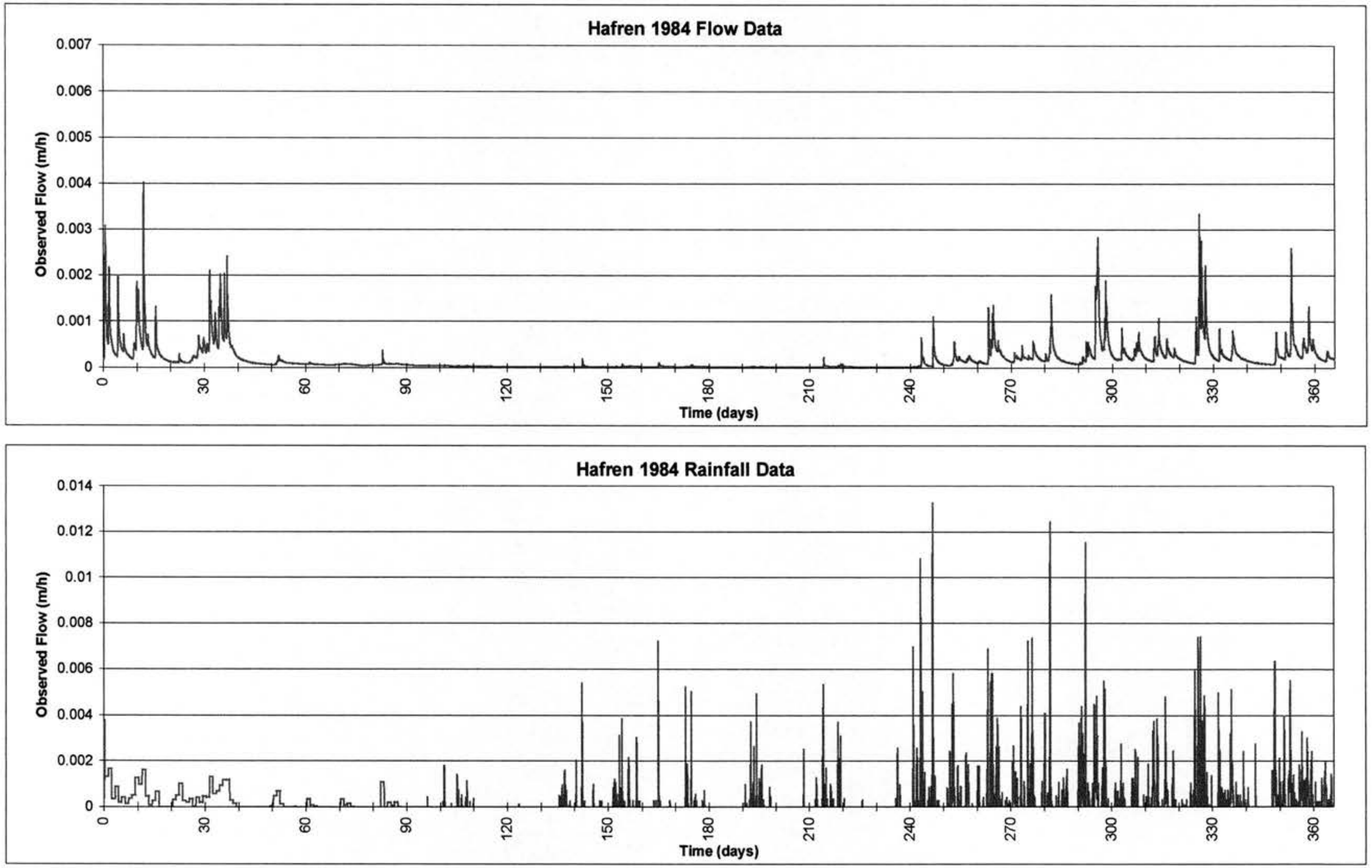
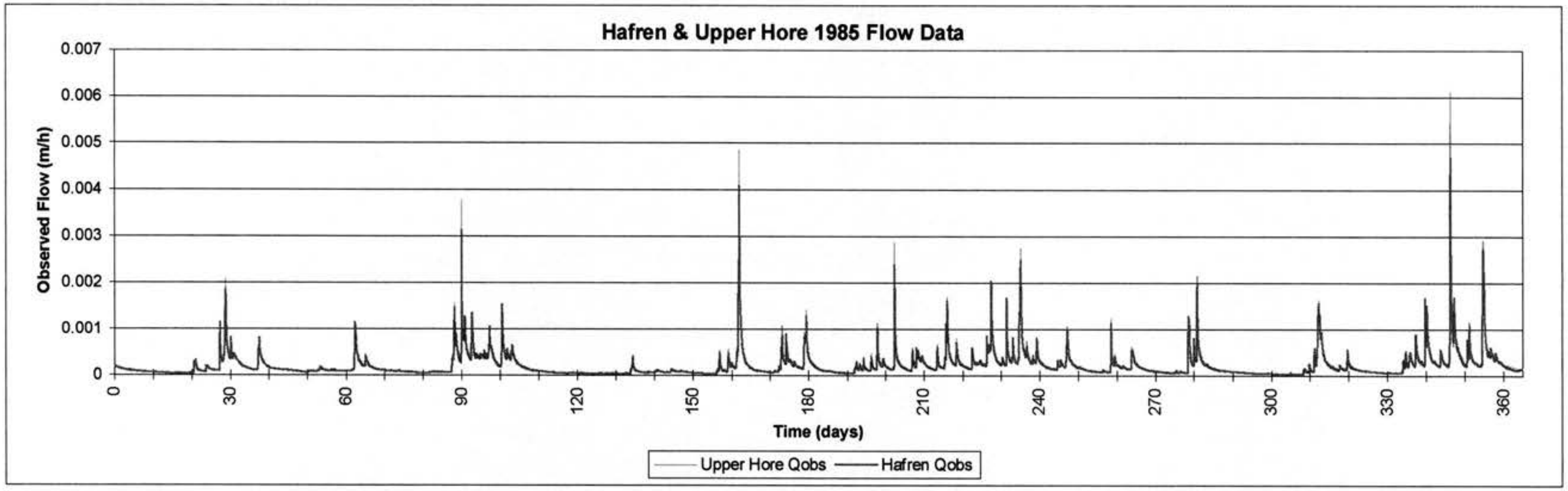


Figure 4.3 – 1984 Flow and Rainfall Data



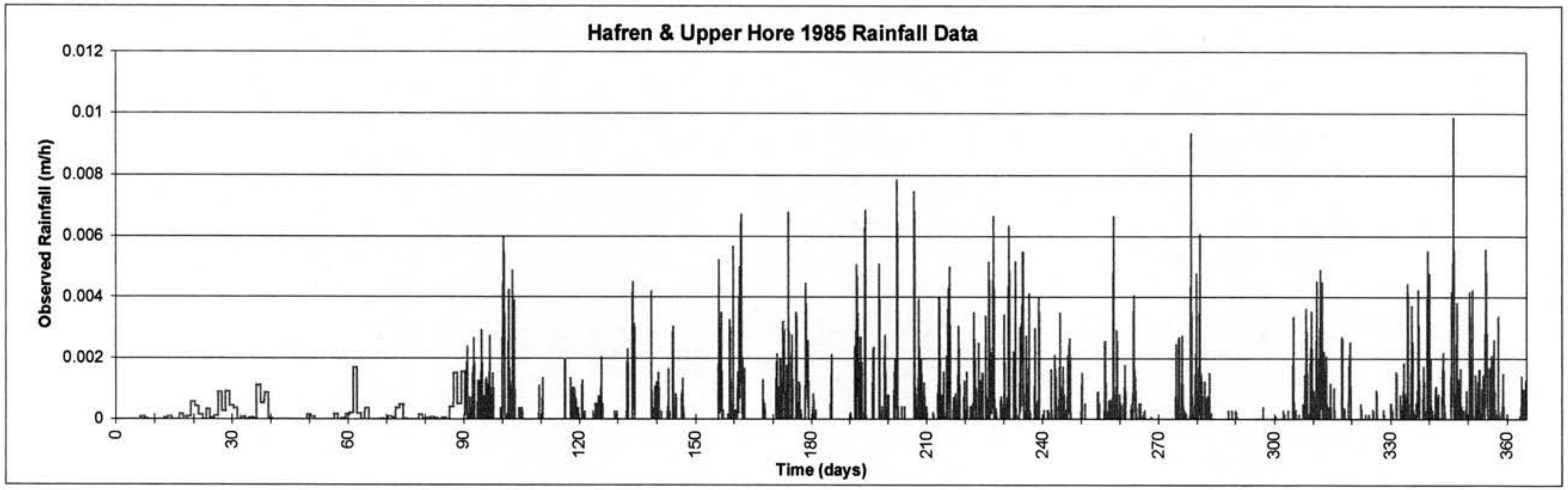


Figure 4.4 – 1985 Flow and Rainfall Data

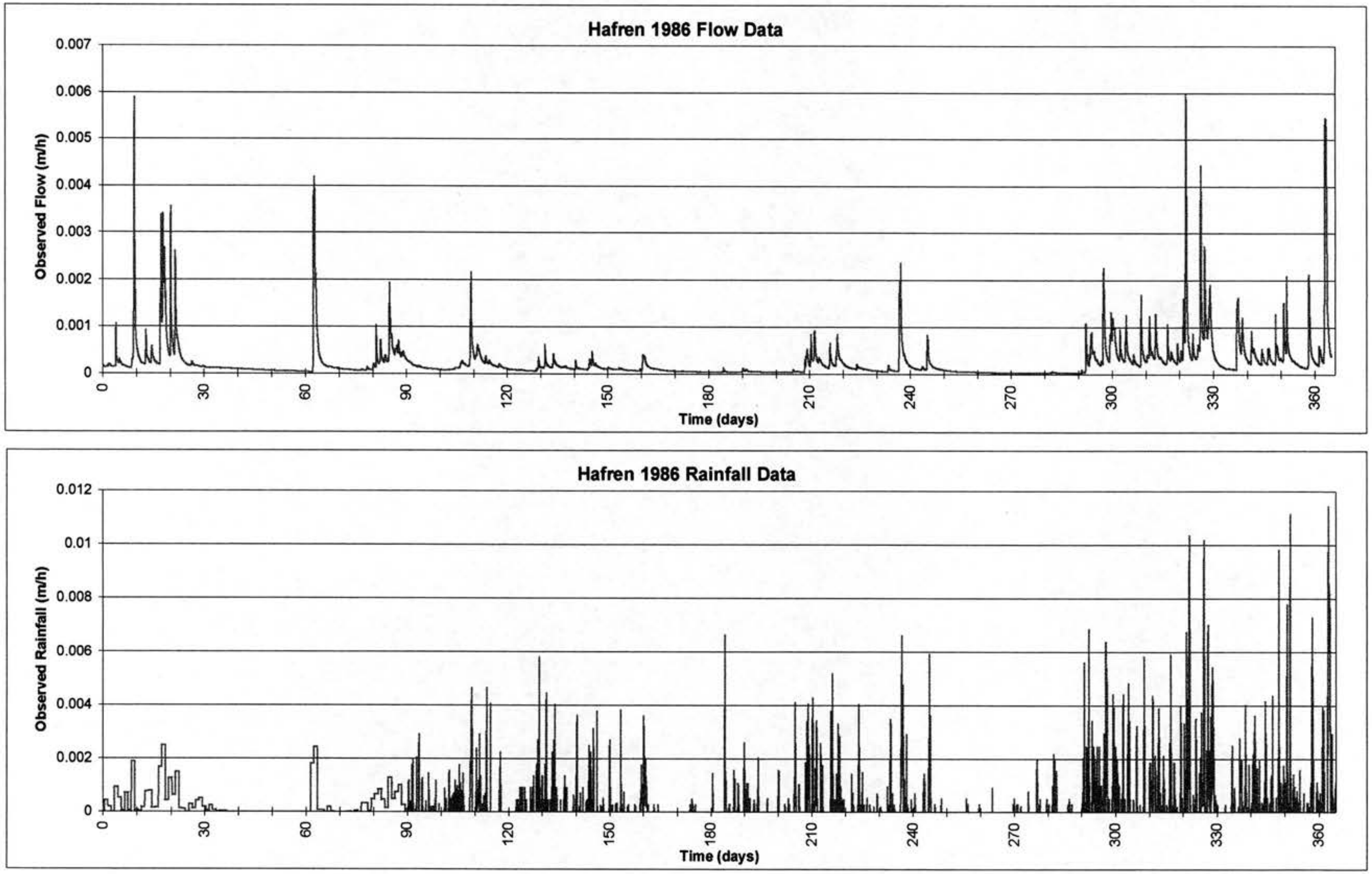


Figure 4.5 – 1986 Flow and Rainfall Data

4.2 Preliminary Evaluation of Model Performance

In order to gain a sense of how TOPMODEL behaved under different parameter combinations for the entire Hafren catchment, some preliminary runs were carried out. In particular these initial simulations focussed on the effect of different m and root zone storage (SRMAX) values[3]. The objective was to evaluate model efficiencies for total catchment outflow over the three years 1984-86. Two values of m were used in these preliminary simulations:

- m = 0.0093 m (Quinn and Beven, 1993)
- m = 0.021 m (Lamb, 1996)

both of which were derived for the Gwy catchment adjacent to the Hafren. The former is a grassland catchment whereas the Hafren is predominantly forested, but the fact that m is representative more of the subsurface storage-discharge processes justified using the same value for the Hafren, given the similar soil types and geological characteristics. The difference between the two published values of m can be attributed to the different modelling approaches. Quinn and Beven (1993) carried out a manual optimisation of m which probably gave greater weight to the flood peaks, whereas Lamb (1996) carried out a statistical analysis of hydrograph recession limbs to obtain a characteristic storage discharge curve for the catchment.

The values of SRMAX used were:

- SRMAX = 0.0899 m (Quinn and Beven, 1993)
- SRMAX = 0.0225 m
- SRMAX = 0.225 m

The two latter values of SRMAX were chosen following some initial testing to consider the effect of decreasing and increasing the root zone and interception losses.

The simulations were carried out using a one hour timestep because, on the basis of the research by Quinn and Beven (1993), it was felt that such a time step would be

[3] The variability of a spatially lumped K0 was not considered at this stage because it would be dealt with later in the research. A value of 889.7419 m/h was used based on Quinn and Beven's (1993) calibrated value of T0 = 8.2746 m^2/h

sufficient to allow the model to simulate the dynamic variations in the saturated contributing areas. The model efficiencies for the different combinations, calculated using Eqn. 3.22, are summarised in Tab. 4.3.

	Hafren 1986		Hafren 1985		Hafren 1984	
m (m)	*0.021*	*0.0093*	*0.021*	*0.0093*	*0.021*	*0.0093*
SRMAX (m)						
0.0225	77.91%	70.67%	60.34%	77.74%	78.25%	57.87%
0.0899	71.00%	64.04%	33.64%	59.23%	75.83%	59.14%
0.225	63.80%	58.73%	16.95%	30.90%	68.18%	52.40%

Table 4.3 - TOPMODEL efficiencies for different m & SRMAX values

The various components of the simulated flows, as summarised in Tab. 4.4 for the 1986 data, were examined to gain a better understanding of the results. Given that this tabular format of presenting results will be used throughout the present chapter, a brief description of its' contents is given below.

CATCHMENT & YEAR *Const. K0 soil distribution*	**HAFREN - 86**	**HAFREN - 86**	**HAFREN - 86**	**HAFREN - 86**	**HAFREN - 86**	**HAFREN - 86**
TOPMODEL Parameters						
m (m)	0.021	0.0093	0.021	0.0093	0.021	0.0093
SRMAX (m)	0.0225	0.0225	0.0899	0.0899	0.225	0.225
SKO (m/h)	889.7419	889.7419	889.7419	889.7419	889.7419	889.7419
T0=m*KO (m^2/h)	18.68	8.27	18.68	8.27	18.68	8.27
Gamma	4.75	5.56	4.75	5.56	4.75	5.56
MODEL EFFICIENCY	**77.91%**	**70.77%**	**70.91%**	**64.01%**	**63.80%**	**58.73%**
FLOW COMP. TOTALS (and % of total sim. flow)						
SAT. ZONE RECHARGE (m)	1.100	1.021	0.955	0.882	0.849	0.782
BASEFLOW (m)	1.062 / 92.47	1.008 / 85.90	0.917 / 92.26	0.868 / 85.23	0.811 / 91.98	0.768 / 84.75
SAT. EXCESS FLOW (m)	0.083 / 7.19	0.143 / 12.23	0.074 / 7.40	0.129 / 12.69	0.067 / 7.63	0.118 / 13.05
SAT. FROM ABOVE (m)	0.004 / 0.34	0.022 / 1.88	0.003 / 0.35	0.021 / 2.08	0.003 / 0.39	0.020 / 2.19
WATER BALANCE						
TOTAL SIMULATED FLOWS (m)	1.149	1.173	0.994	1.018	0.882	0.907
TOTAL OBSERVED FLOWS (m)	1.339	1.339	1.339	1.339	1.339	1.339
TOTAL RAINFALL (m)	1.743	1.743	1.743	1.743	1.743	1.743
TOTAL POTENTIAL ET (m)	1.057	1.057	1.057	1.057	1.057	1.057
TOTAL PREDICTED ET (m)	0.556	0.556	0.711	0.711	0.823	0.823
FINAL BALANCE (m)	0.000	0.000	0.000	0.000	0.000	0.000

Table 4.4 - Summary of TOPMODEL Performance for Preliminary Runs

The results for each simulation are represented as separate columns. In each column the first three lines are the values of m, SRMAX and K_0 used in the simulation. These are then followed by the calculated spatially lumped value of T_0, together with the value of the average catchment soil-topographic index (gamma), and finally the model efficiency. This latter value is the primary indicator of how well TOPMODEL is simulating the total catchment response.

The second block of data in the table summarises how TOPMODEL is simulating the breakdown of the various flow components into

- saturated zone recharge
- baseflow
- saturation excess flow
- saturation from above flow

For each of the components, the total volumes for the simulation period are given, as well as the percentage of total observed flow. These data were particularly useful given that they provided a more detailed picture of how well the model was simulating the various components in the transformation of rainfall to runoff. With regards to the saturation from above flow component, it is an artifact of TOPMODEL that allows the representation of runoff from catchment cells that become saturated during the course of a simulation timestep (see Paragraph 3.3.1).

When examining the flow component values for the various simulations, the reader should bear in mind that they are expressed as flows per unit area. Given a total catchment area of 8,657,117m^2, small variations in flow components up to 10^{-3}m will correspond to flow volumes of the order of 10^3 cubic metres.

Finally, the last block of data contains the summary values for the entire simulation period. In particular, it is useful to compare the total simulated flows to the total observed flows, as well as the predicted evapotranspiration against the potential evapotranspiration which is derived from field measurements. The final balance is calculated by summing all the precipitation, runoff, evapotranspiration and storage components and, assuming a lack of deep groundwater fluxes, should ideally always be zero over a calendar year. It is therefore useful for verifying that over a chosen simulation period TOPMODEL is not predicting losses or accumulation of water within the catchment. This may not always be the case for single event simulations.

Again, the reader should bear in mind that all of the above volumes are expressed per unit area.

From the results summarised in Tab. 4.4, it can be observed that a decrease in SRMAX produced a noticeable increase in model efficiency, accompanied by an increase in the total simulated flows. The reduction in SRMAX was also accompanied by a significant decrease in the total predicted evaporation, which was largely accounted for by an increase in the saturated zone recharge.

With regard to the m parameter, the model efficiencies did not show a consistent trend though it must be underlined that the range of variability of m was significantly less than that of SRMAX. As a general observation, a decrease in m was associated with a decrease in baseflow and an increase in the saturated flow components.

Overall then, it is clear that within a wide range of possible values of m and SRMAX the performance of TOPMODEL can vary significantly.

4.3 Identification of Optimal Parameter Set

The wide variations in efficiency values found during the preliminary simulations justified the need to carry out an optimisation of model parameters. Furthermore, in order to evaluate the effect of spatial soil variability what was needed was a base case with spatially uniform K_0. Given the availability of flow data for the Upper Hore catchment only for the year 1985, it was decided that this year would be used to represent the base case parameters for the Hafren catchment.

An optimal parameter set was identified by selecting a first random set of 1000 different combinations of m, SRMAX and K_0 values and iteratively running TOPMODEL through all of them. The model efficiencies found for this first iteration ranged from 58% to 85%, with roughly 150 parameter combinations giving efficiencies above 80%. It was therefore decided to select a narrower range of parameter values associated with a cut-off efficiency of 80% and recalculate a second random set of 1000 parameter sets. From this second set, a narrower range of (m, SRMAX, K_0) was selected by choosing a cut-off efficiency of 85% and a third random set was recalculated. The parameter set that then gave the highest efficiency in this third optimisation was then chosen. The ranges used in the three successive 1000 run iterations are summarised in Tab. 4.5.

	Optimisation no.1	Optimisation no.2	Optimisation no.3
m (m)	0.01-0.1	0.01-0.014	0.01295-0.01362
SRMAX (m)	0.001-0.1	0.006-0.26	0.00603-0.0069
K_0 (m/hr)	885-895	885-895	886.436-893.292

Table 4.5 - Parameter ranges used in optimisation with constant K_0

The final parameter set chosen from the third optimisation was

m = 0.0132 m; SRMAX = 0.00616 m; K_0avg = 890.978 m/hr

which provided an efficiency of 85.19% for the 1985 simulation period. The parameter K_0avg represents the calibrated lumped lateral saturated conductivity. The corresponding value of T0, for the chosen m and K_0avg, is equal to 11.7609m^2/h. It should be noted that repeating the above optimisation procedure with an initial range of K_0 = 1-1000 m/h led to efficiencies greater than 85% for K_0 = 870 – 916 m/h. This indicates that the choice of initial K_0 values did not affect the optimal parameter set.

To validate these parameter values, they were also applied to the the 1984 and 1986 Hafren data, as well as to the 1985 Upper Hore data. The results of these simulations are summarised in Tab. 4.6 and the relative hydrographs are shown in Figs. 4.6, 4.7. The time step used for these, and all subsequent simulations was again equal to one hour. The appropriateness of such a value will be re-evaluated in Chapter 5 on the basis of the spatial soil moisture deficit predictions.

CATCHMENT & YEAR *Const. K0 Soil Distribution*	HAFREN 1985	UPPER HORE 1985	HAFREN 1986	HAFREN 1984
TOPMODEL Parameters				
m (m)	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616
KO (m/h)	890.978	890.978	890.978	890.978
T0=m*KO (m^2/h)	11.761	11.761	11.761	11.761
Gamma	5.304	4.993	5.304	5.304
MODEL EFFICIENCY	**85.40%**	**85.20%**	**84.96%**	**72.92%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW				
SAT. ZONE RECHARGE (m)	0.933	0.946	1.211	0.859
BASEFLOW (m)	.956 / 90.33	.969 / 89.20	1.189 / 88.82	.853 / 102.46
SAT. EXCESS FLOW (m)	.078 / 7.40	.065 / 5.96	.125 / 9.36	.074 / 8.86
SAT. FROM ABOVE (m)	.004 / .39	.004 / .40	.011 / .85	.006 / .66
WATER BALANCE				
TOTAL SIMULATED FLOWS (m)	1.039	1.038	1.326	0.933
TOTAL OBSERVED FLOWS (m)	1.058	1.086	1.339	0.833
TOTAL RAINFALL (m)	1.431	1.431	1.743	1.284
TOTAL POTENTIAL ET (m)	1.009	1.009	1.057	1.271
TOTAL PREDICTED ET (m)	0.415	0.415	0.395	0.349
FINAL BALANCE (m)	-0.001	-0.001	0.000	-0.005

Table 4.6 - Summary of Catchment Results

The chosen parameter set gave very similar efficiencies for the Hafren 1986 and Upper Hore 1985 simulations. For these cases the hydrograph plots consistently show a good match between Qobs and Qsim, both in the flood peaks and in the recession limbs. For the Hafren in 1984 there is a significant reduction in efficiency, associated with an overestimation of flows in the latter part of the year and a visibly worse match to Qobs.

The main points to note from these simulations are that:

a) the efficiencies for Hafren 1985 and Upper Hore 1985 are very similar;

b) in the different simulation years similar efficiency values can be obtained with different flow component percentages;

c) the baseflow component percentages for 1985-86are all around 90%. Given the high precipitation and runoff associated with the Hafren, which corresponds to protracted periods of soil saturation, it is surprising that the saturated flow component percentages are not higher.

All of the above points will be further examined in the following chapter.

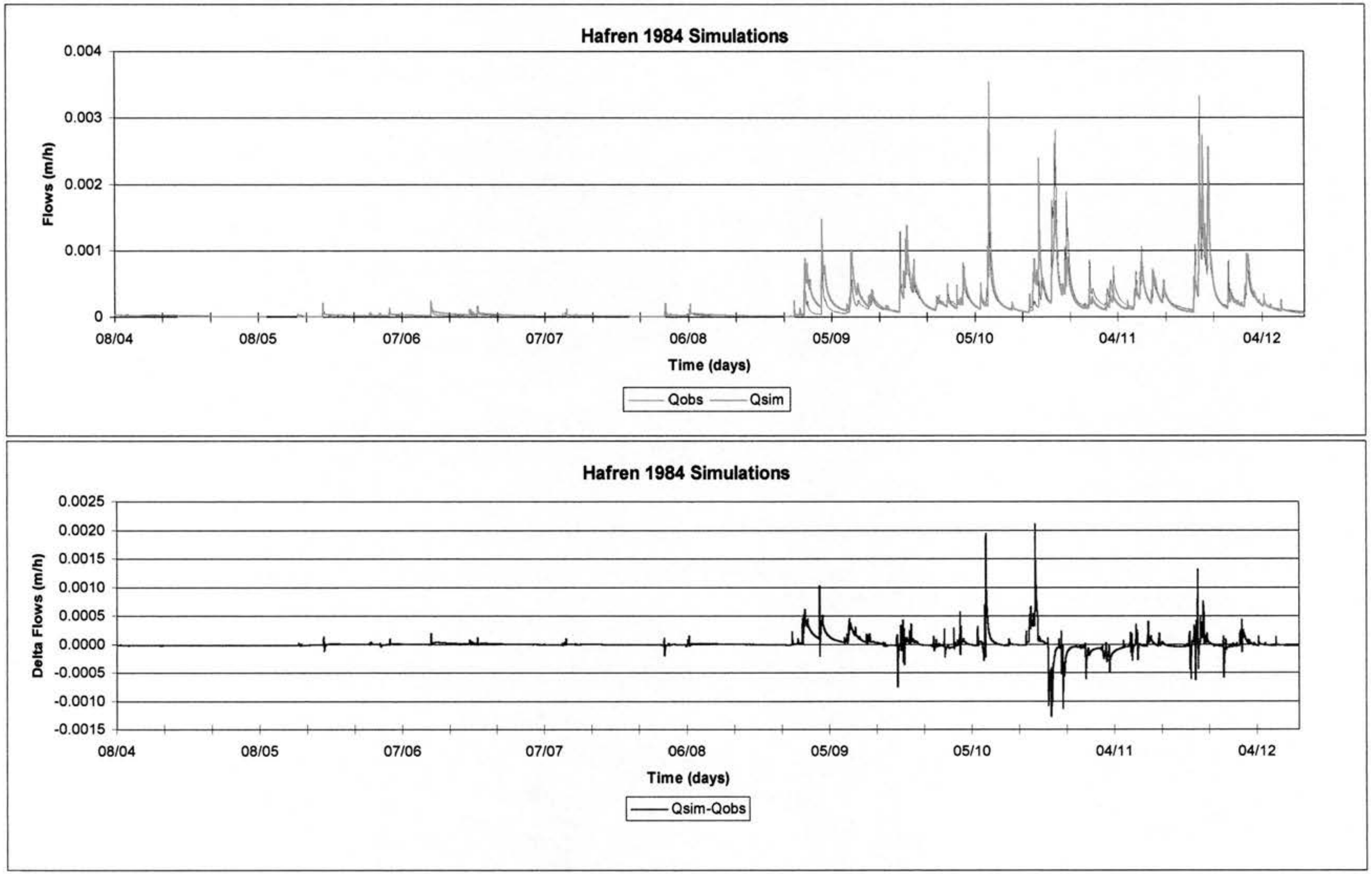


Figure 4.6a - 1984 Hafren Simulations with Constant K0

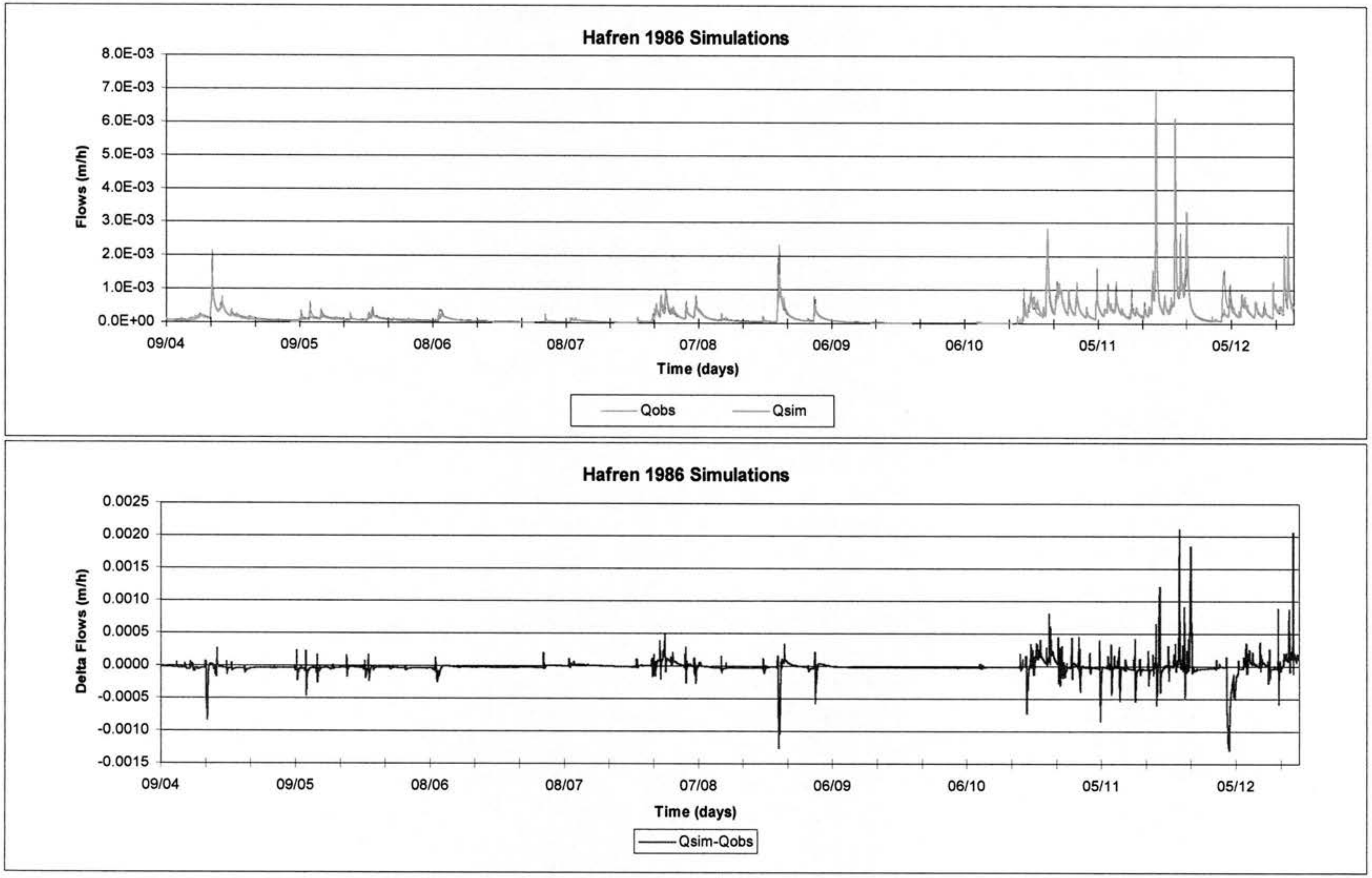


Figure 4.6b - 1986 Hafren Simulations with Constant K0

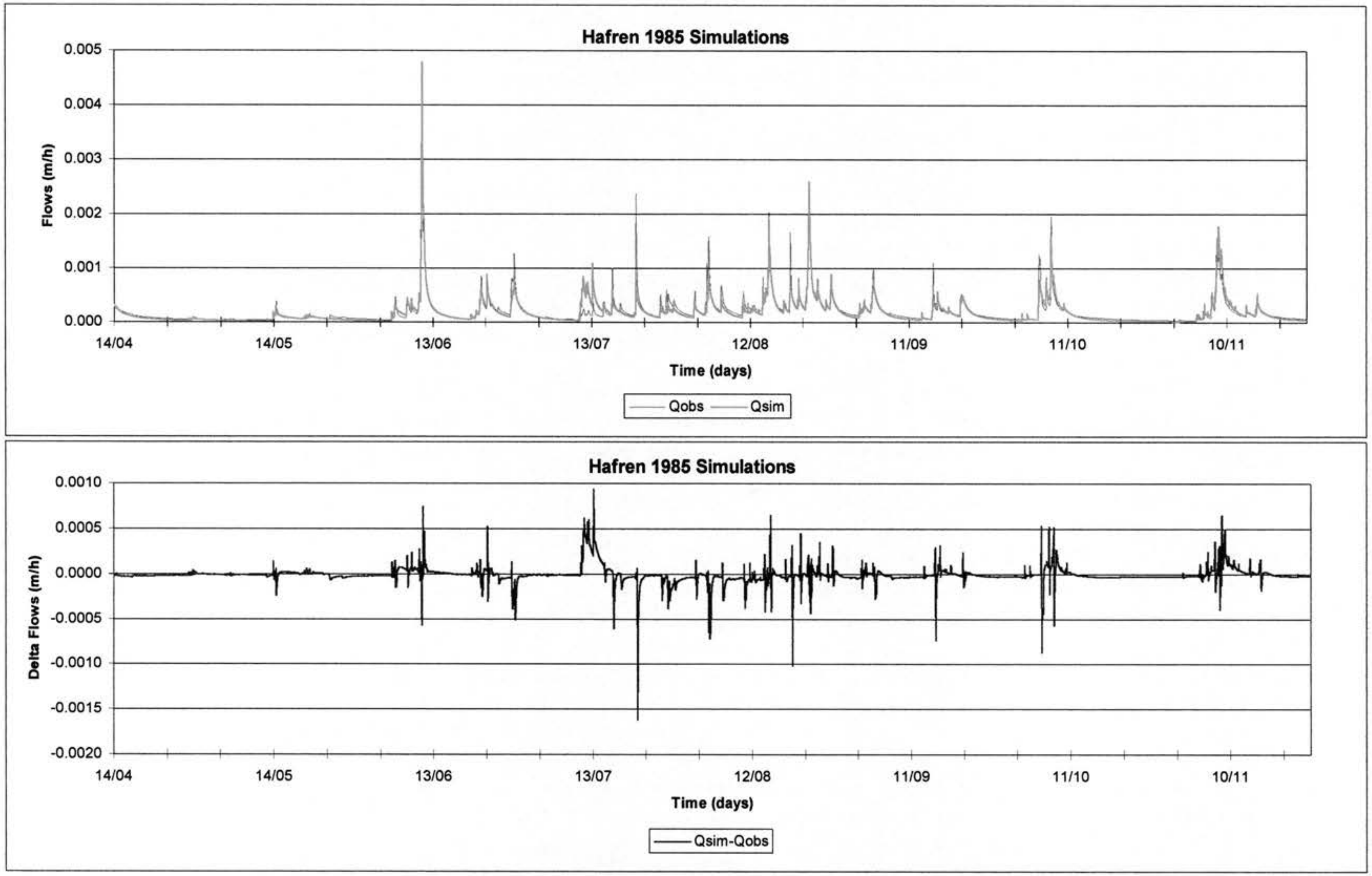


Figure 4.6c - 1985 Hafren Simulations with Constant K0

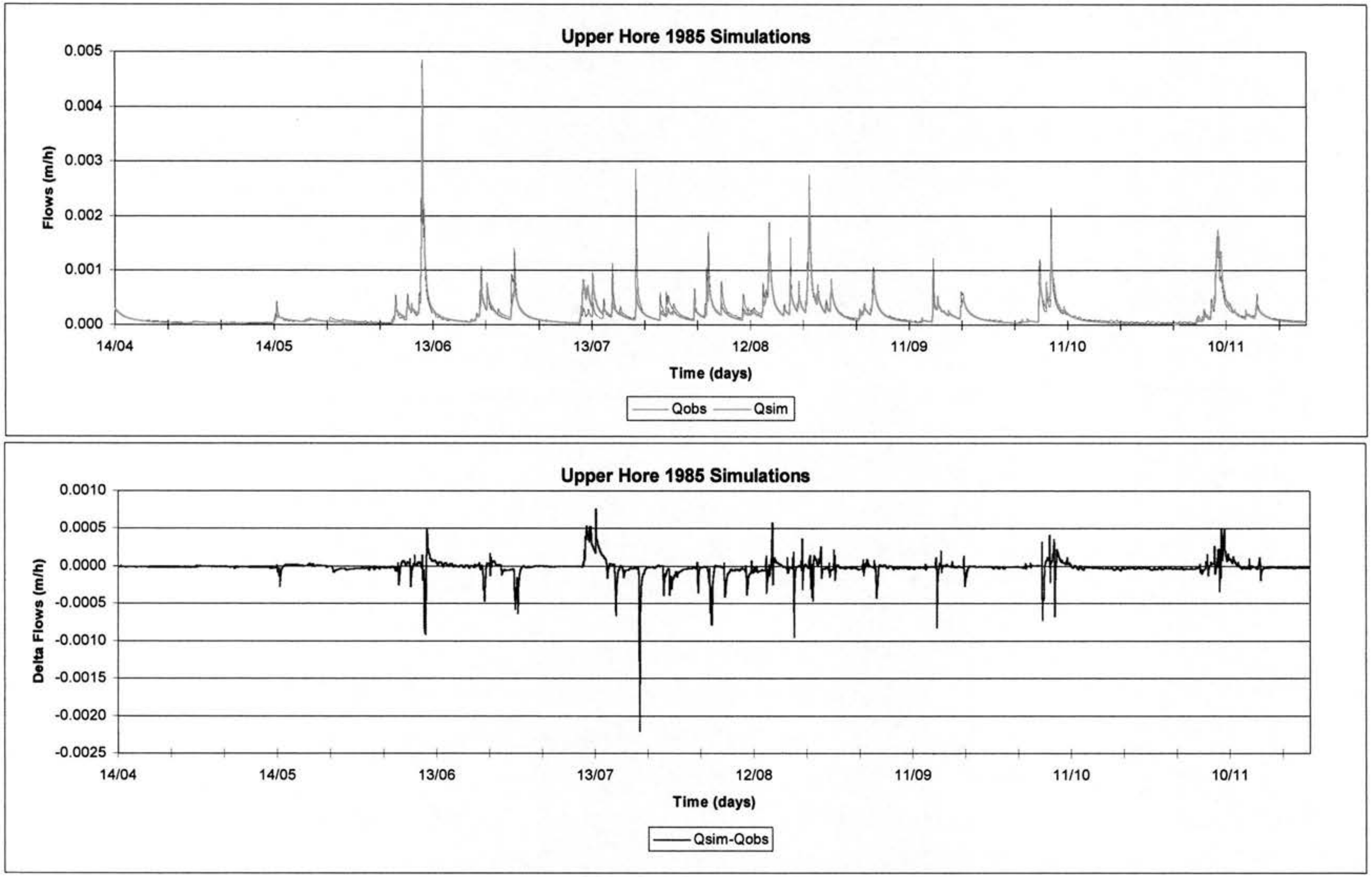


Figure 4.6d - 1985 Upper Hore Simulations with Constant K0

4.4 Simulations with Published Saturated Conductivities

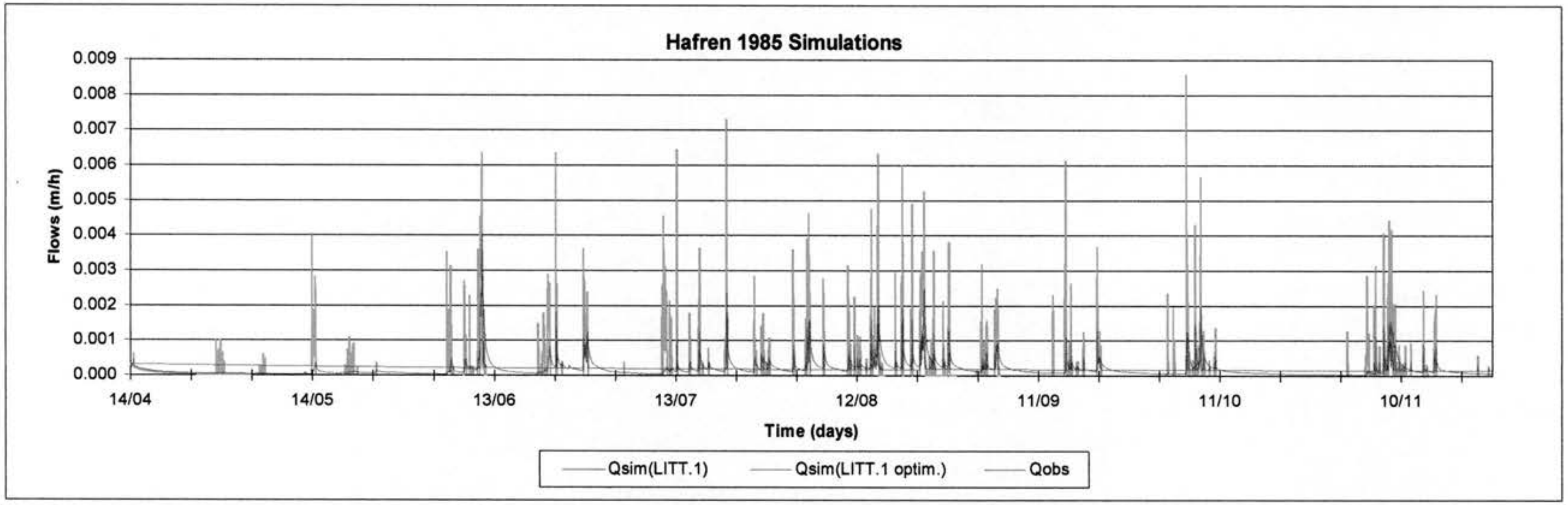
Having identified an optimal parameter set and the associated base case for a spatially uniform K_0avg, the next step involved using realistic distributions of K_0 based on published data. The two distributions used, based on the LITT.1 and LITT.2 classifications, have already been described in the previous chapter.

The simulations with the two soil distributions are summarised in Tab. 4.7[4] which clearly indicates that the realistic values of K_0 - roughly 3 orders of magnitude smaller than K_0avg - gave unacceptable results. The reasons why the difference between the two sets of values is so large will be examined further in the following chapter. Though, coincidentally, the volume of total simulated flows is very close to that of the total observed flows for both distributions, the flow components show a very different representation of catchment processes. The two distributions both show a dominant flow contribution due to saturation excess flow and this is confirmed by the hydrograph plots in Fig. 4.8.

CATCHMENT & YEAR *Soil Distribution*	HAFREN - 85 *Const. K0*	HAFREN - 85 *LITT. 1*	HAFREN - 85 *LITT. 2*	HAFREN - 85 *LITT. 1 Optim.*	HAFREN - 85 *LITT. 2 Optim.*
TOPMODEL Parameters					
m (m)	0.0132	0.0132	0.0132	0.88026	0.98458
SRMAX (m)	0.00616	0.00616	0.00616	0.12743	0.15666
KO (m/h)	890.978	n.a.	n.a.	n.a.	n.a.
T0=m*KO (m^2/h)	11.761	0.009	0.005	0.588	0.400
Spatially Avg. KO	n.a	0.667823	0.406416	0.667823	0.406416
Gamma	5.212	12.565	13.234	8.364	8.924
MODEL EFFICIENCY	**85.40%**	**-387.60%**	**-417.17%**	**25.99%**	**7.51%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW					
SAT. ZONE RECHARGE (m)	0.933	0.095	0.067	0.431	0.324
BASEFLOW (m)	.956 / 90.33	.133 / 12.59	.109 / 10.31	1.075 / 101.56	1.077 / 101.76
SAT. EXCESS FLOW (m)	.078 / 7.40	.906 / 85.63	.932 / 88.04	.180 / 16.99	.265 / 25.04
SAT. FROM ABOVE (m)	.004 / .39	.014 / 1.34	.017 / 1.59	.000 / .02	.000 / .00
WATER BALANCE					
TOTAL SIMULATED FLOWS (m)	1.039	1.054	1.058	1.255	1.342
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058	1.058	1.058
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.820	0.842
FINAL BALANCE (m)	-0.001	-0.001	-0.001	-0.001	-0.001

Table 4.7 - Simulations with Published K_0 Distributions

[4] In this table there is an additional data value in the first block which indicates the calculated area weighted average of K_0. Also, the values shown for T_0 in the LITT.1 and LITT.2 columns are the calculated area weighted averages evaluated from the m and $K_0(x,y)$ values of each cell.



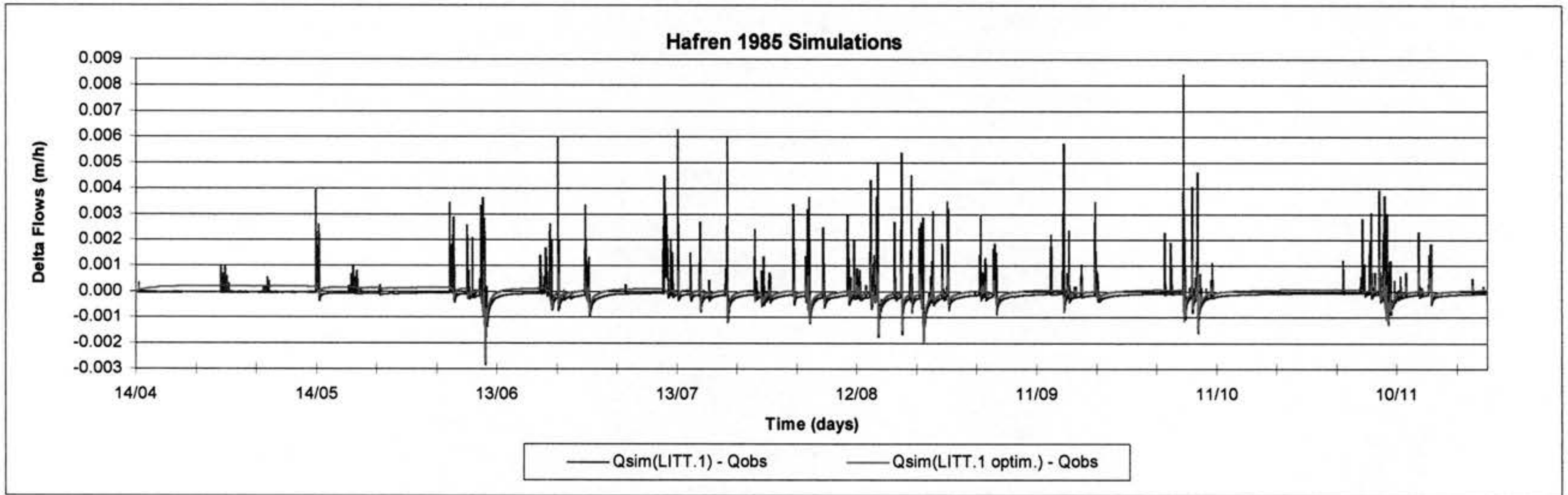
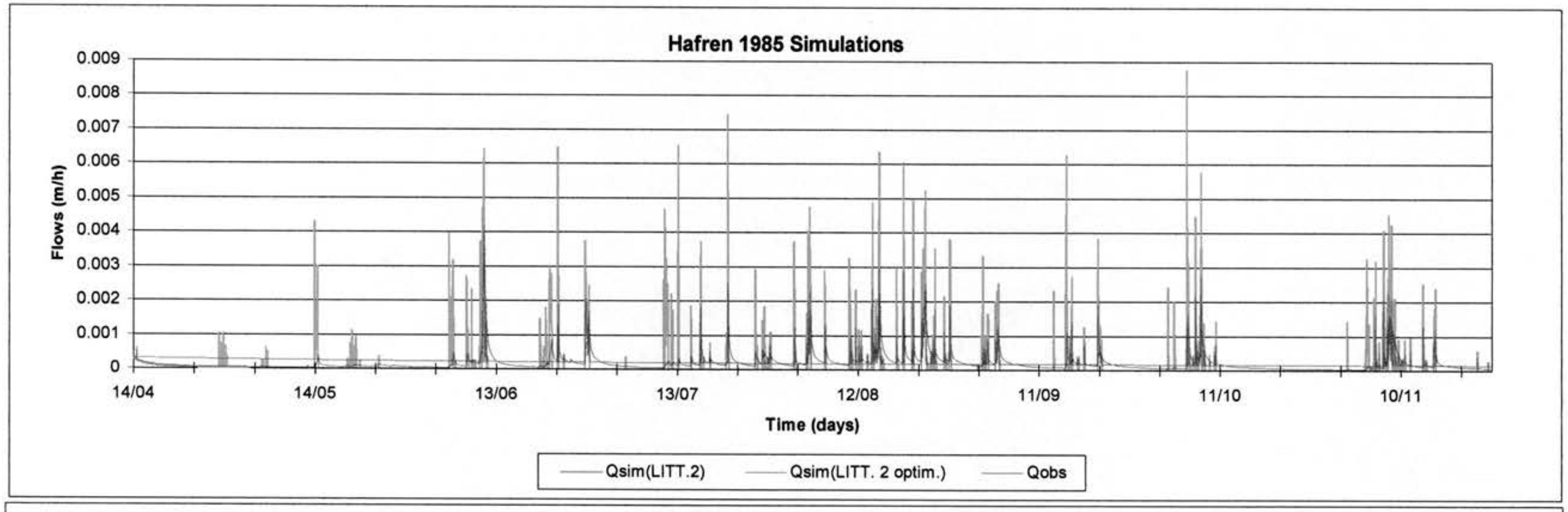


Figure 4.8a - Hafren Simulations with LITT.1 K0



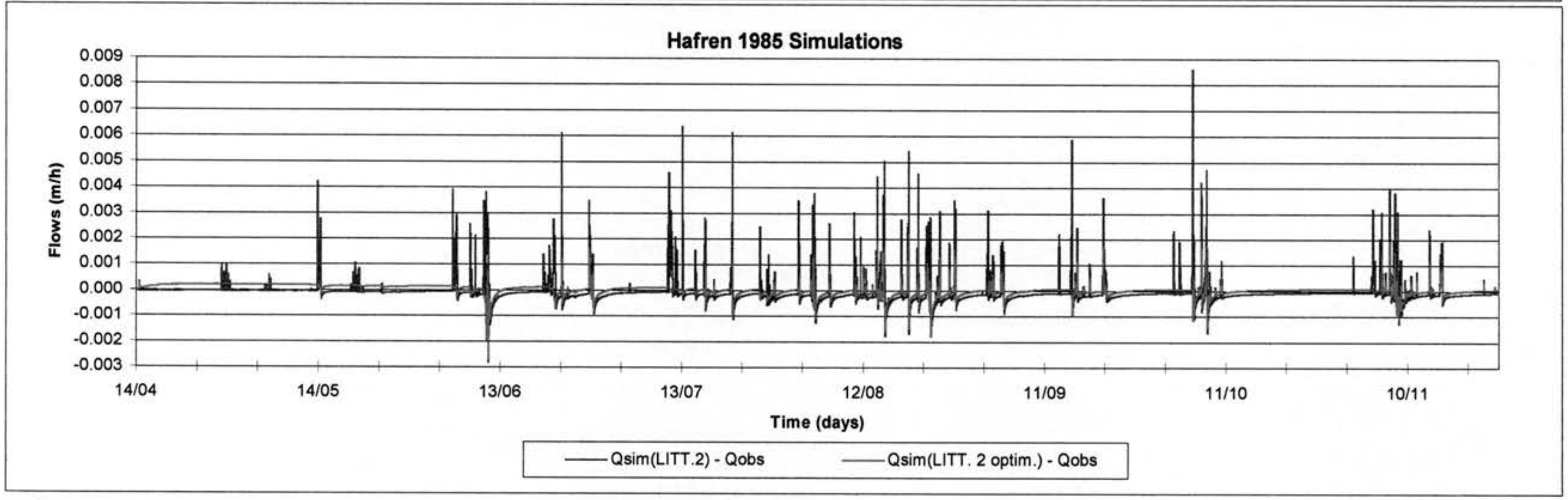


Figure 4.8b - Hafren Simulations with LITT.2 K0

To evaluate if a recalibration of (m, SRMAX) parameters could modify the distribution of component flows, it was decided to re-optimise these two parameters. By increasing the initial range of variability of m and SRMAX - and thus enlarge the parameter space - it was hoped that the optimisation procedure described in Section 4.3 would provide more acceptable parameter values, while still allowing the use of the published K_0 values. The initial ranges selected for m and SRMAX are summarised in Tab. 4.8

	LITT.1 K_0	LITT.2 K_0
m (m)	0.001 - 1.0	0.001 - 1.0
SRMAX (m)	0.001 - 1.0	0.001 - 1.0

Table 4.8 - Initial ranges used in optimisations with LITT.1 & LITT.2

Though the new optimised parameter sets did give more sensible efficiencies and flow component percentages (see Tab. 4.7 , they led to a significant overestimation in the total simulated flows. An examination of the hydrograph plots (see Fig. 4.8) also shows that the effect of the new parameter sets has simply been to shift the baseflow component upward, but overall the match is no better. The increase in baseflow can be attributed to the very high values of m which, as shown in Section 3.3.1, controls the catchment storage-discharge mechanism which directly affects baseflow.

From the above results we can therefore conclude that even by reoptimising, the new model parameters (m, SRMAX) are actually less meaningful in terms of the resulting hydrographs and, therefore, the use of published K_0 values does not lead to acceptable model results with TOPMODEL.

4.5 Simulations with Scaled Saturated Conductivities

4.5.1 Hafren catchment simulations

Given the results obtained with the unaltered K_0 distributions in the previous paragraph, it was necessary to identify a solution that would allow TOPMODEL to incorporate spatially variable soil data, while still providing sensible hydrograph simulations. The solution identified involved normalising all K_0 distributions so that their spatial average would always be equal to the lumped calibrated K_0avg. This was obtained by multiplying the each value of K_0 - or of the proxy-index used - by a scaling factor equal to

$$K_{0corr} = \frac{K_0 avg}{average[K_0(x,y)]} \qquad \text{(Eqn. 4.1)}$$

where the denominator (average[$K_0(x,y)$]) is the area weighted average calculated for the chosen distributions and shown in Tab. 4.1. The scaled values of K_0 for each soil type together with the corresponding $\ln(T_0)$ value are summarised in Tab. 4.9. From this table we can also see that for the Crowdy, Hafren, Skiddaw and Wilcock soils, which cover 99% of the Hafren catchment, the scaled K_0 values for the HOST SPR distribution are quite similar to the calibrated value of K_0avg. This therefore implies that almost all of the catchment soils will show a behaviour - in terms of scaled K_0 - which is not radically different from the case of constant K_0.

			LITT. 1		LITT. 2		Wetness Class		HOST BFI		HOST SPR	
Soil	Symbol	Area (sq.m)	Scaled K0	ln(T0)	Scaled K0	ln(T0)	Scaled K0	ln(T0)	Scaled K0	ln(T0)	Scaled K0	ln(T0)
Aled	Aj	17500	58.838	-0.253	96.647	0.244	164.417	0.775	2720.544	3.581	400.930	1.666
Crowdy	Cj	3887500	803.321	2.361	1320.024	2.858	986.505	2.567	578.115	2.032	962.231	2.542
Hafren	HN	2970000	803.321	2.361	289.386	1.340	822.087	2.384	1292.258	2.837	769.785	2.319
Manod	Mj	47500	74.048	-0.023	102.451	0.302	164.417	0.775	2040.408	3.293	465.078	1.815
Skiddaw	Skd	995000	803.321	2.361	1320.024	2.858	822.087	2.384	884.177	2.457	962.231	2.542
Wilcock	Wo	740000	1893.895	3.219	544.633	1.973	822.087	2.384	816.163	2.377	946.194	2.525
Area weighted average			**891.026**		**891.030**		**890.964**		**890.972**		**890.981**	
Calibrated K0avg:			**890.978**									
ln(m*K0avg):			**2.465**									

Note
- The scaled component of the soil-topographic index is calculated as: ln(T0) = ln(m*K0), where m = 0.0132.

Table 4.9 - Summary of Rescaled K_0 Values: Hafren Catchment

A direct comparison between the different K0 distributions is not possible given the very different methods with which they were all derived. But if we examine the tabular data and the plot of normalised K_0 against soil types in Fig. 4.9, the following important aspects are observed:

a) the scaled Wetness Class and HOST-SPR curves are very similar;
b) the scaled LITT.2 curve shows the same shape as the HOST-SPR curve, but with a greater range of variability;

c) the scaled LITT.1 curve is generally similar to the HOST-SPR curve, except for the Wilcock soil which is showing a higher scaled K_0 value.

d) the HOST-BFI curve is essentially inverted with respect to all the other curves, and this is due to the complementary relationship between baseflow and surface runoff. Given that we are interested in simulating runoff generating processes, the HOST-BFI curve is of little relevance and will not be used for the simulations.

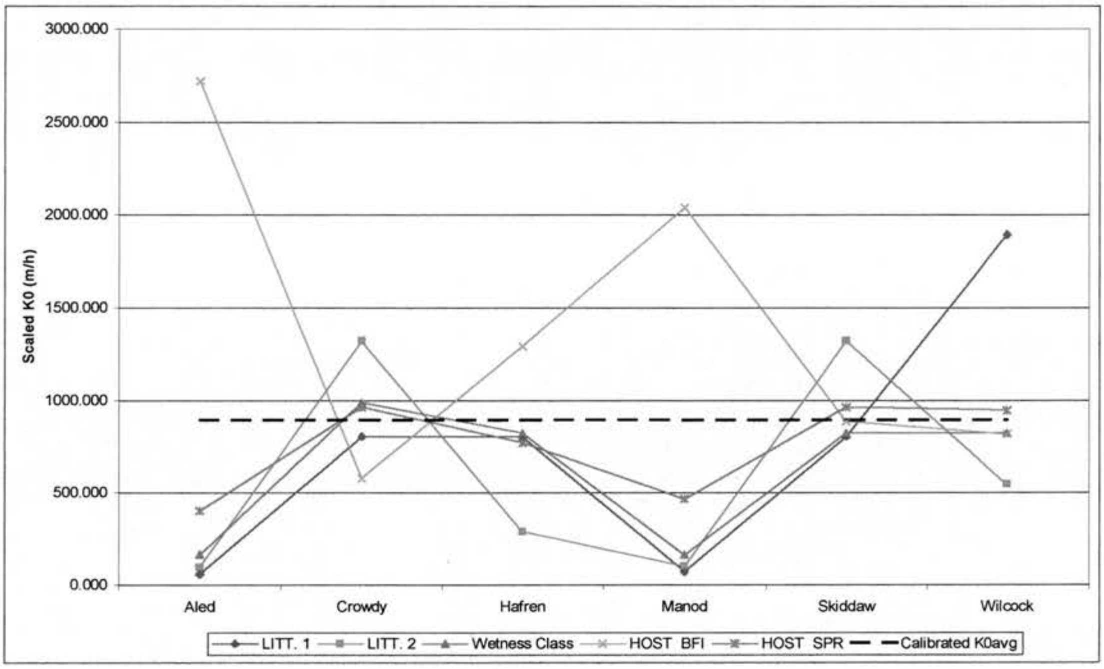


Figure 4.9 - Scaled K_0 values

On the basis of the above comparison, we can therefore state that all of the distributions - except the HOST-BFI - are generally consistent with one another. It is therefore not possible to exclude any of them a priori, except for the HOST-BFI. The performance of TOPMODEL with each of the distributions will therefore be considered to identify the most appropriate one for the Hafren catchment.

The simulations with the selected K_0 distributions were carried out for the 1985 data, for which the results are summarised in Tab. 4.10. The simulations were also carried out for the 1984 and 1986 data in order to validate the results, and the efficiencies obtained are also shown. The table below shows that in all cases the maximum efficiencies are still given by the constant K_0 case, though the difference in efficiency with respect to the worst distribution is never more than 2%. The K_0 distributions that give the best results in 1985 are Litt.1, Wetness Class and HOST-SPR, with the latter being the best distribution over all three years. If we examine the plots of the distribution functions in Fig. 4.10 we can see that this is due to the fact that the curves for the above three distributions are those most similar to the curve for a spatially uniform K_0.

CATCHMENT & YEAR *Soil Distribution*	HAFREN - 85 *Const. K0*	HAFREN - 85 *LITT. 1*	HAFREN - 85 *LITT. 2*	HAFREN - 85 *Wetness Class*	HAFREN - 85 *HOST-SPR*
TOPMODEL Parameters					
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	890.978	890.978	890.978	890.978
T0=m*KO (m^2/h)	11.7609	11.7618	11.7618	11.7610	11.7610
Spatially Avg. K0 (m)	n.a	891.026	891.030	890.964	890.981
Gamma	5.212	5.370	5.543	5.328	5.328
EFFICIENCY '85	**85.40%**	**85.20%**	84.87%	85.19%	**85.20%**
EFFICIENCY '86	**84.96%**	84.60%	83.64%	84.73%	**84.77%**
EFFICIENCY '84	**72.92%**	72.35%	71.16%	72.53%	**72.58%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW					
SAT. ZONE RECHARGE (m)	0.933	0.924	0.914	0.924	0.924
BASEFLOW (m)	.956 / 90.33	.947 / 89.51	.938 / 88.60	.947 / 89.51	.947 / 89.52
SAT. EXCESS FLOW (m)	.078 / 7.40	.087 / 8.18	.096 / 9.08	.087 / 8.21	.087 / 8.19
SAT. FROM ABOVE (m)	.004 / .39	.005 / .44	.005 / .45	.004 / .42	.004 / .42
WATER BALANCE					
TOTAL SIMULATED FLOWS (m)	1.039	1.039	1.039	1.039	1.039
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058	1.058	1.058
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.415	0.415
FINAL BALANCE (m)	-0.001	-0.001	-0.001	-0.001	-0.001

Table 4.10 - Simulations with Scaled K_0 Distributions

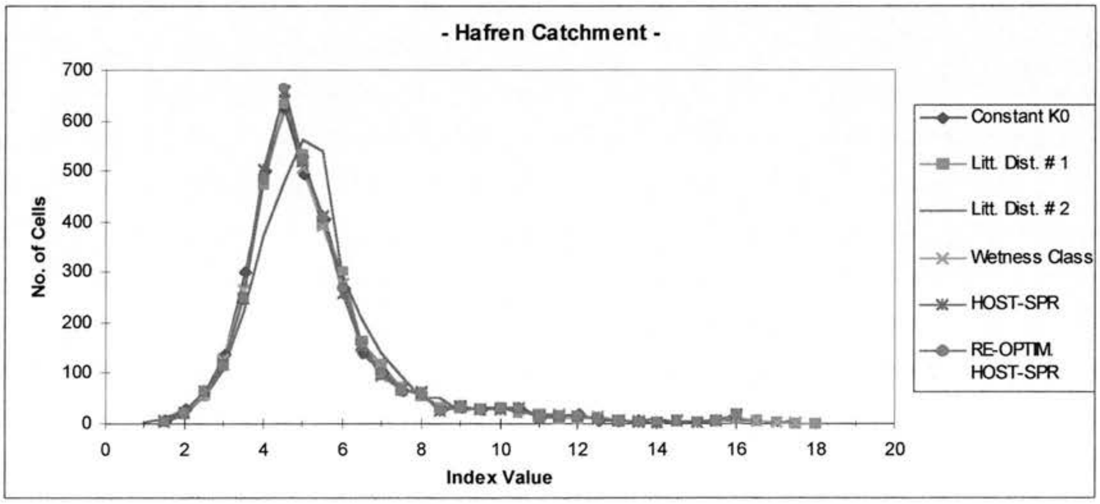


Figure 4.10 - Comparison of Soil-Topographic Index Distributions

If we consider the differences in the actual calculated flows for the Hafren 1985 data (Fig. 4.11), we can see that the constant K_0, the LITT.1 and the HOST-SPR calculated flows (Qsim) are virtually identical. In the hydrographs we can also see that the match to the observed flows (Qobs) is very good throughout the year, and especially in the latter half once the catchment has wetted up after the drier summer period.

To verify if the optimal values of (m, SRMAX) were affected by the chosen soil distribution, the iteration procedure described in Section 4.3 was carried out again, with K_0avg being used to calculate a scaling parameter for the spatially distributed HOST-SPR K_0. Given that the optimisation results for LITT.1 and LITT.2 clearly showed that widening the initial range did not lead to better model predictions (Tab. 4.7 this justified choosing the same initial ranges as used in Section 4.3. All of the optimisation steps are summarised in Tab. 4.11

	Optimisation no.1	Optimisation no.2	Optimisation no.3
m (m)	0.01-0.1	0.01043-0.01554	0.0119-0.01434
SRMAX (m)	0.001-0.1	0.00634-0.2502	0.00639-0.00865
K_0 (m/hr)	885-895	885.49-894.258	885.705-894.114

Table 4.11 - Parameter ranges used in successive optimisations

The final parameter set chosen from the third iteration was

- m = 0.01321 m
- SRMAX = 0.0064 m
- K_0 = 888.989 m/hr

which gave an efficiency of 85.17% with respect to predicted outflows (Tab. 4.12).

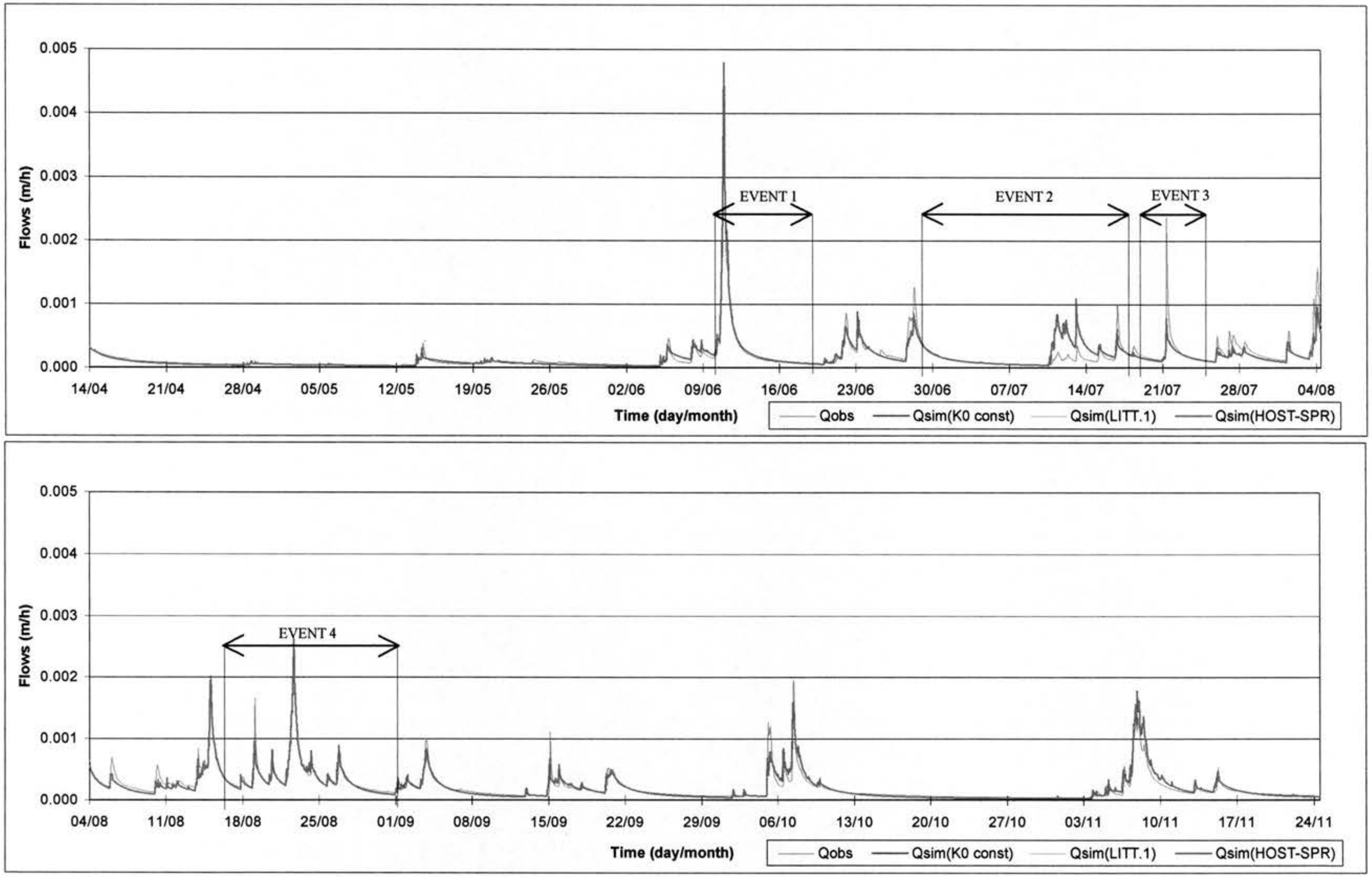


Figure 4.11a - Hydrographs for Diff. Scaled K0 Classifications - Hafren 1985

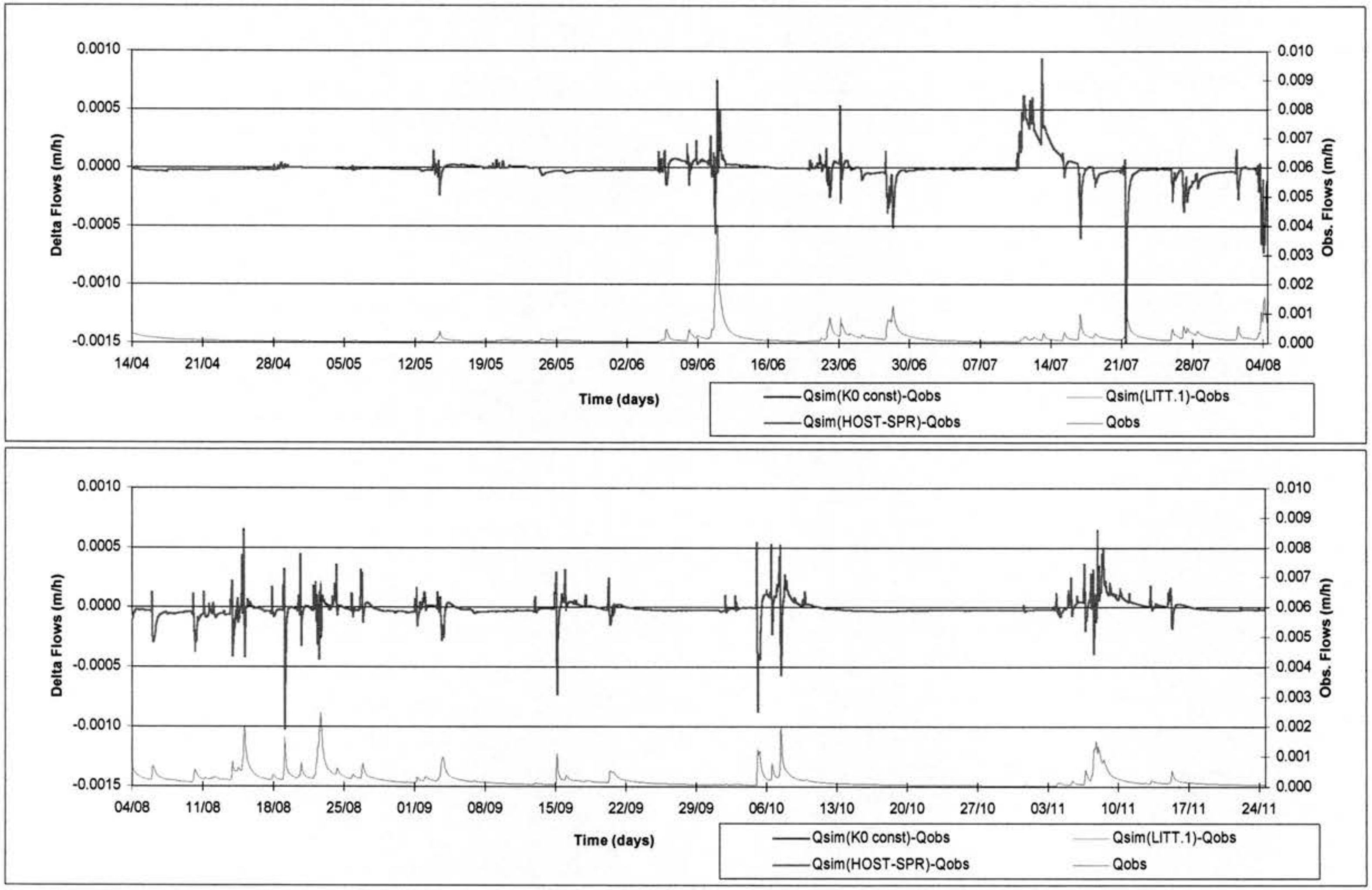


Figure 4.11b - Hydrographs for Diff. Scaled K0 Distributions - Hafren 1985

The same parameter set was used with the 1984 and 1986 Hafren data, and the efficiencies were 72.28% and 84.51% respectively. By comparing against the efficiencies of the original optimised parameter set it is therefore clear that the re-optimised (m, SRMAX, K_0avg) parameters actually give slightly worse results set over all three simulation periods, even though in terms of the breakdown into the various flow components there is no noticeable change.

CATCHMENT & YEAR	**HAFREN - 85**	**HAFREN - 85**	**HAFREN - 85**
Soil Distribution	***Const. K0***	***HOST-SPR***	***Re-optimised HOST-SPR***
TOPMODEL Parameters			
m (m)	0.0132	0.0132	0.01321
SRMAX (m)	0.00616	0.00616	0.0064
K0 (m/h)	890.978	890.978	888.989
T0=m*KO (m^2/h)	11.7609	11.7610	11.7437
Spatially Avg. K0 (m)	n.a	890.981	888.979
Gamma	5.212	5.328	5.329
EFFICIENCY '85	**85.40%**	**85.20%**	**85.17%**
EFFICIENCY '86	**84.96%**	**84.77%**	**84.51%**
EFFICIENCY '84	**72.92%**	**72.58%**	**72.28%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW			
SAT. ZONE RECHARGE (m)	0.933	0.924	0.920
BASEFLOW (m)	.956 / 90.33	.947 / 89.52	.943 / 89.16
SAT. EXCESS FLOW (m)	.078 / 7.40	.087 / 8.19	.086 / 8.16
SAT. FROM ABOVE (m)	.004 / .39	.004 / .42	.004 / .41
WATER BALANCE			
TOTAL SIMULATED FLOWS (m)	1.039	1.039	1.034
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058
TOTAL RAINFALL (m)	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.420
FINAL BALANCE (m)	-0.001	-0.001	-0.001

Table 4.12 - Simulations with Reoptimised Parameter sets: Hafren

Based on the above results we can therefore conclude that the HOST SPR K_0, with the initial optimisation values of (m, SRMAX, K_0avg), provides the best simulation results for the Hafren.

4.5.2 Upper Hore subcatchment simulations

Considering only the 1985 simulation period, the simulations described above for the Hafren were repeated for the Upper Hore using only the final parameter set selected above. The results are summarised in Tab. 4.13 while the hydrographs are shown in Fig. 4.12. As with the Hafren, the global efficiencies are of the order of 85%, and the breakdown of the various component flows is very similar with the Upper Hore showing a slightly higher ratio of baseflow to total saturated flow (13.61 for the Upper Hore vs 10.41 for the Hafren). This can be explained by the fact that the Upper Hore gamma values are all slightly lower than those of the Hafren. This therefore reduces the likelihood of saturation throughout the catchment. The only other difference with respect to the Hafren is that the Litt. 2 soil distribution performs slightly better than both the Litt. 1 distribution and the HOST-SPR distribution.

CATCHMENT & YEAR ***Soil Distribution***	**UPPER HORE - 85** ***Const. K0***	**UPPER HORE - 85** ***LITT. 1***	**UPPER HORE - 85** ***LITT. 2***	**UPPER HORE - 85** ***Wetness Class***	**UPPER HORE - 85** ***HOST-SPR***
TOPMODEL Parameters					
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	890.978	890.978	890.978	890.978
T0=m*KO (m^2/h)	11.761	11.761	11.763	11.761	11.761
Spatially Avg. K0 (m)	n.a.	890.977	891.132	890.987	890.976
Gamma	4.993	5.003	5.152	5.008	5.008
EFFICIENCY '85	**85.20%**	85.20%	**85.40%**	85.17%	**85.19%**
EFFICIENCY HAFREN '85	**85.40%**	85.20%	**84.87%**	85.19%	**85.20%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW					
SAT. ZONE RECHARGE (m)	0.946	0.945	0.933	0.944	0.945
BASEFLOW (m)	.969 / 89.20	.967 / 89.08	.956 / 88.01	.967 / 89.03	.967 / 89.05
SAT. EXCESS FLOW (m)	.065 / 5.96	.066 / 6.11	.077 / 7.11	.067 / 6.17	.067 / 6.15
SAT. FROM ABOVE (m)	.004 / .40	.004 / .37	.005 / .44	.004 / .36	.004 / .37
WATER BALANCE					
TOTAL SIMULATED FLOWS (m)	1.038	1.038	1.038	1.038	1.038
TOTAL OBSERVED FLOWS (m)	1.086	1.086	1.086	1.086	1.086
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.415	0.415
FINAL BALANCE (m)	-0.001	-0.001	-0.001	-0.001	-0.001

Table 4.13 - Simulations with Scaled K_0 Distributions: Upper Hore

These results therefore indicate that in terms of predicted outflows, the inclusion of a spatially variable K_0 does not significantly affect the results at the subcatchment scale.

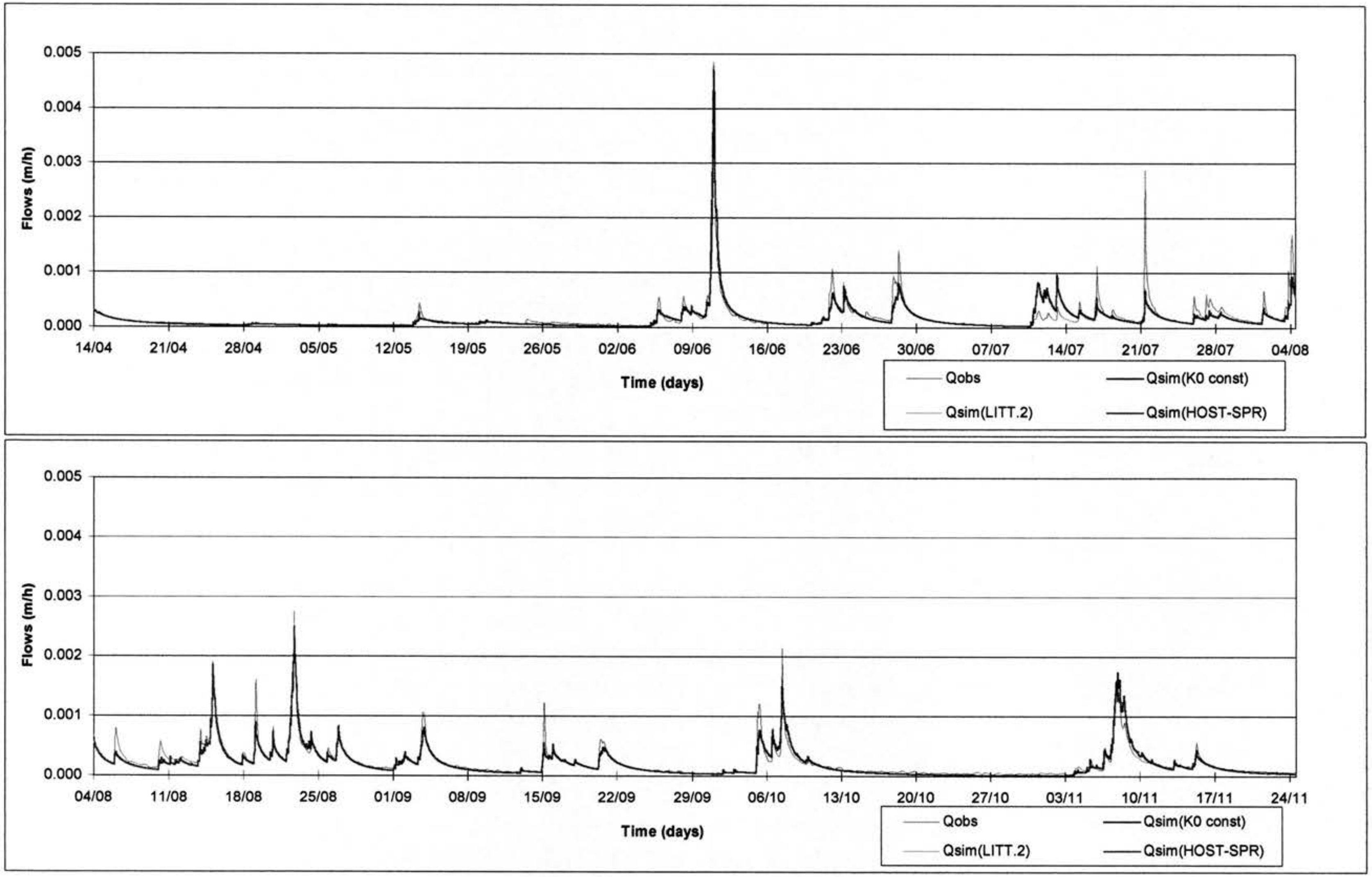


Figure 4.12a - Hydrographs for Diff. Scaled K0 Distributions - Upper Hore 1985

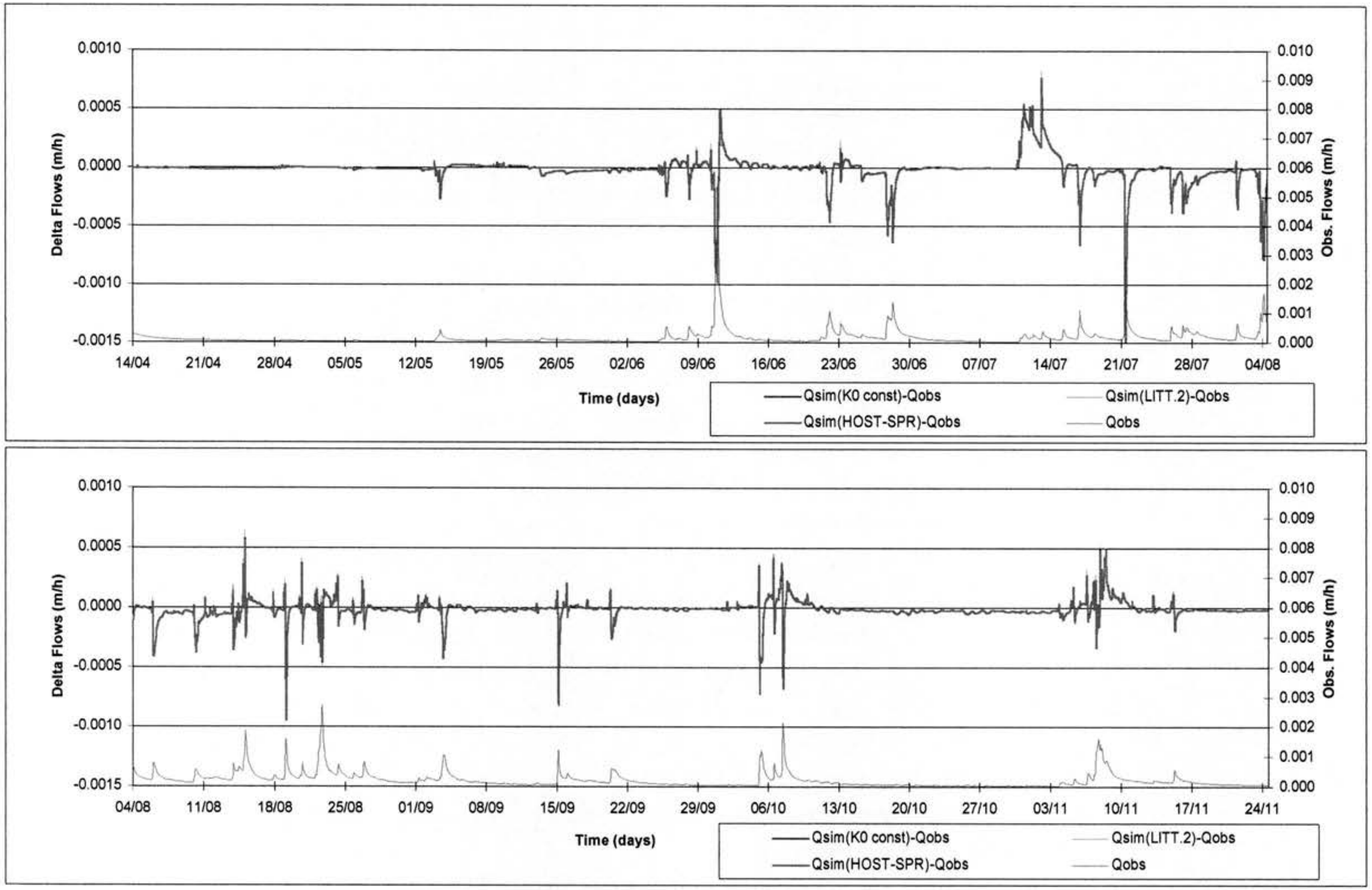


Figure 4.12b - Hydrographs for Diff. Scaled K0 Distributions - Upper Hore 1985

4.5.3 Choice of a Spatial K_0 Distribution

For the purpose of comparing the results obtained with a constant K_0 against those obtained with a single spatially variable distribution, it was necessary to select a single spatially variable K_0 distribution which would be used in all the remaining simulations.

On the basis of the results obtained for the Hafren and the Upper Hore, it was decided to exclude from subsequent simulations:

a) the LITT.1 and LITT.2 distributions because they do not relate to TOPMODEL's interpretation of K_0, as confirmed by the results in Section 4.4;
b) the Wetness Class which - though very similar to the HOST-SPR K_0 distribution - was felt to be less representative given that it does not account for soil storage capacity in any way, nor does it consider the range of soil properties that are accounted for in the HOST classification.

Given that the HOST-SPR index values were derived from actual runoff data, it was felt that the subsequent single event and SMD simulations would provide the ideal opportunity to evaluate it's suitability for catchment modelling applications.

4.5.4 Simulations considering a channel initiation threshold

Given that the use of spatially distributed soil saturated conductivities had very little effect on the predicted outflow, both for the Hafren catchment and the Upper Hore subcatchment, it was decided to carry out additional simulations making use of the channel initiation threshold variable (CIT) as described by Quinn et al. (1995a). As pointed out in the previous chapter, the treatment of river cells in the calculation of the topographic index can have a significant impact on the index distribution and, consequently, on the catchment average value of gamma. Before proceeding with the successive stages of the simulation it seemed appropriate to consider this aspect in more detail.

Various values of CIT were considered and the resulting topographic index distributions for the Hafren are shown in Fig. 4.13. It should be remembered that

CIT_∞ indicates that the CIT value is greater than the catchment area and therefore no cell can ever be a drainage network cell.

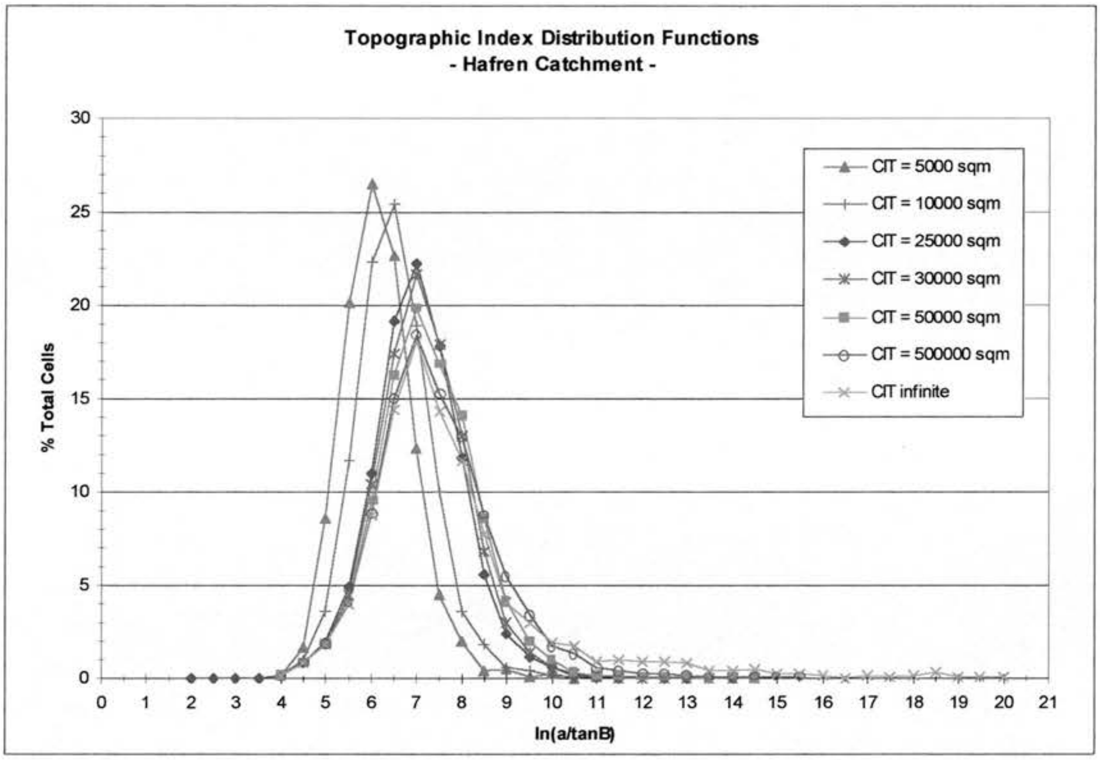


Figure 4.13 - Hafren Topographic Index Distributions for varying CIT

It is clear from the graph that above CIT = 25000 m^2 the distribution curves are quite similar. Following the interpretation given by Quinn et al. (1995a), 25000 m^2 is the CIT value which is considered to most accurately reflect the actual catchment drainage network. Using this value for both the Hafren and the Upper Hore, two modified topographic index distributions were recalculated assuming:

1) Method 1: the modified definition of topographic index proposed by Quinn et al. (1995a), for the cells having CIT > 25000 m^2. To calculate the modified topographic index the geometrical configuration shown in Fig. 4.14 is adopted, where A is the total upslope area and L is the channel length equal to the grid size.

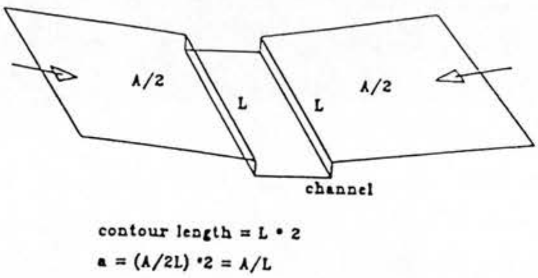


Figure 4.14 - Geometric Schematisation of River Cells
(from Quinn et al., 1995a)

2) Method 2: that all river cells would be removed from the topographic index distribution.

The resulting distributions obtained for the Hafren and the Upper Hore are shown below in Fig. 4.15, 4.16. Looking at the figures various conclusions can be drawn.

1) It is evident that for both catchments the differences in the topographic index distributions calculated with the two different methods are minor, and are essentially concentrated in the lower-middle range of index values.
2) If we compare the soil-topographic index distributions curves for the two catchments to the case of infinite CIT, there are two significant differences. For both catchments the Method1 (M1) and Method2 (M2) curves present higher peaks and a more compact distribution with respect to the CIT infinite curves. The M1 and M2 modified distributions will therefore result in smaller values of gamma, as is shown in Tab. 4.14.

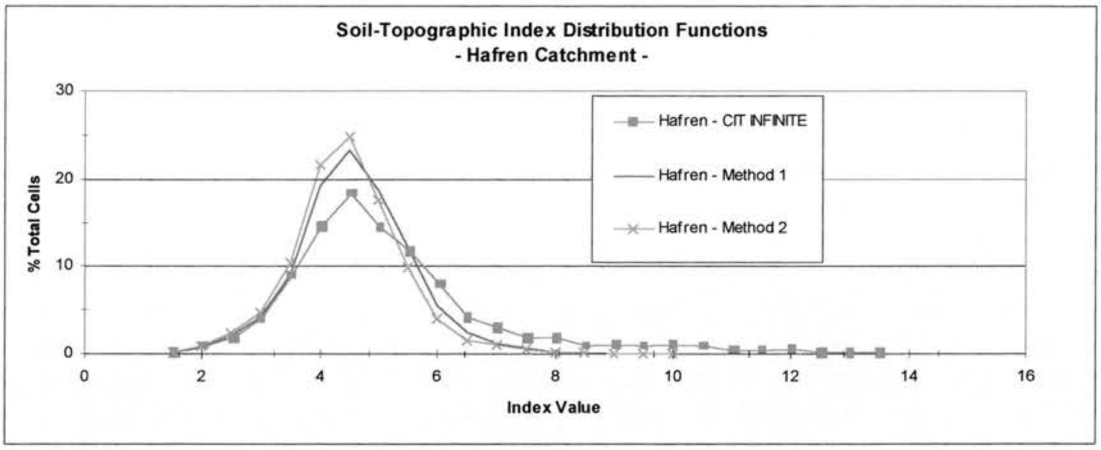


Figure 4.15 - Hafren Modified Soil-Topographic Index Distributions

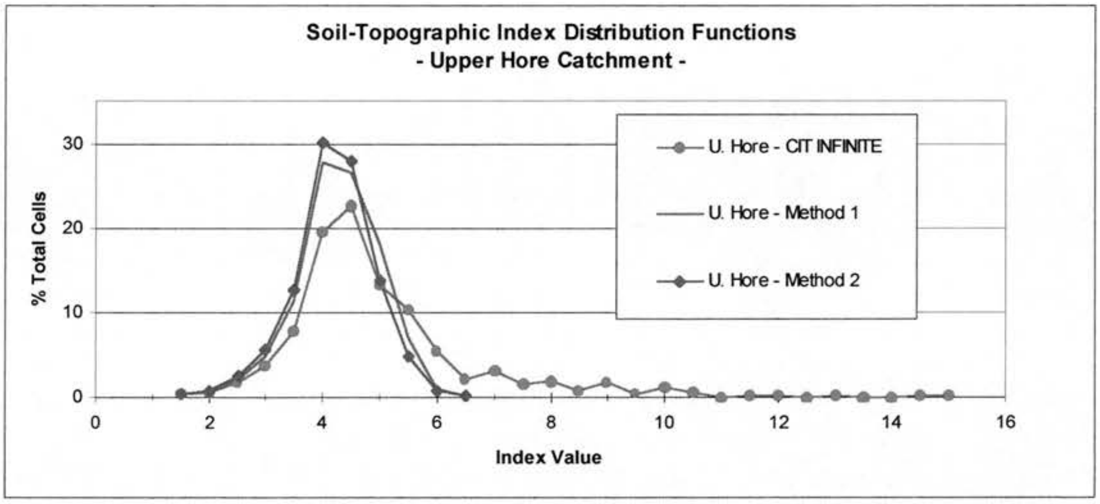


Figure 4.16 - Upper Hore Modified Soil-Topographic Index Distributions

The TOPMODEL simulations were carried out again for the 1985 period and the results are shown in Tab. 4.14 while the hydrographs are shown in Figs. 4.17, 4.18.

It is clear from examining the results that modifying the calculation of the topographic index to account for the river cells has a noticeable effect on the model efficiencies and on the flow component breakdown. Nonetheless, the results and the hydrographs do show that:

CATCHMENT & YEAR (K0 HOST SPR) *CIT = 25000 sq.m.*	HAFREN - 85 *CIT INFINITE*	HAFREN - 85 *Method 1*	HAFREN - 85 *Method 2*	UPPER HORE - 85 *CIT INFINITE*	UPPER HORE - 85 *Method 1*	UPPER HORE - 85 *Method 2*
TOPMODEL Parameters						
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	890.978	890.978	890.978	890.978	890.978
T0=m*K0 (m^2/h)	11.7610	11.7610	11.7197	11.7609	11.7609	11.7535
Spatially Avg. K0 (m)	890.9811	890.9811	887.8453	890.9764	890.9764	890.4153
Gamma	5.328	4.604	4.483	5.008	4.279	4.184
EFFICIENCY	**85.20%**	**83.18%**	**83.00%**	**85.19%**	**81.19%**	**81.07%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW						
SAT ZONE RECHARGE (m)	0.924	1.004	1.006	0.945	1.014	1.015
BASEFLOW (m)	.947 / 89.52	1.027 / 97.01	1.029 / 97.18	.967 / 89.05	1.036 / 95.44	1.037 / 95.47
SAT. EXCESS FLOW (m)	.087 / 8.19	.009 / .85	.008 / .74	.067 / 6.15	.001 / .07	.001 / .05
SAT. FROM ABOVE (m)	.004 / .42	.003 / .25	.002 / .18	.004 / .37	.000 / .04	.000 / .03
WATER BALANCE						
TOTAL SIMULATED FLOWS (m)	1.039	1.038	1.038	1.038	1.038	1.038
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058	1.086	1.086	1.086
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.415	0.415	0.415
FINAL BUDGET (m)	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001

Table 4.14 - Summary of Simulations using CIT Method

a) the application of the two CIT-based methods has actually resulted in a decrease of 2-4% in model efficiency, accompanied by a 7-8% increase in the baseflow component;

b) the two modified topographic index distributions lead to a global catchment response which is practically identical. This is confirmed by the fact that the calculated cumulative difference between the two hydrographs is equal to $3x10^{-8}$m for the entire simulation period.

c) there appears to be a slight improvement in terms of the spiky nature of the predicted flows, with respect to the results calculated with the standard TOPMODEL (see Figs. 4.12, 4.13).

We can therefore conclude that considering a CIT value of 25000 m^2 did not have a significant effect on the model outflow predictions.

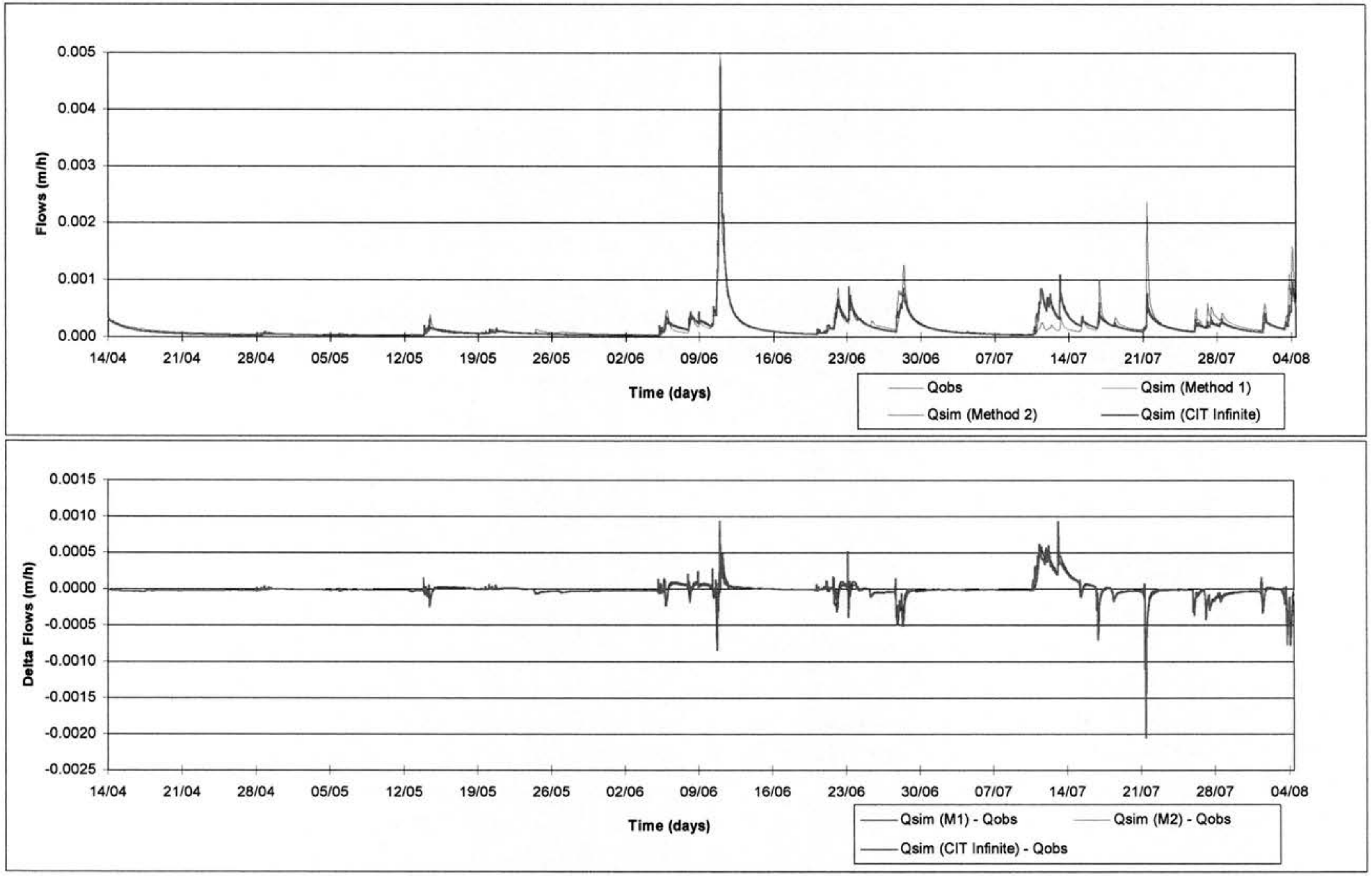


Figure 4.17a - Hydrographs obtained with CIT Methods - Hafren 1985

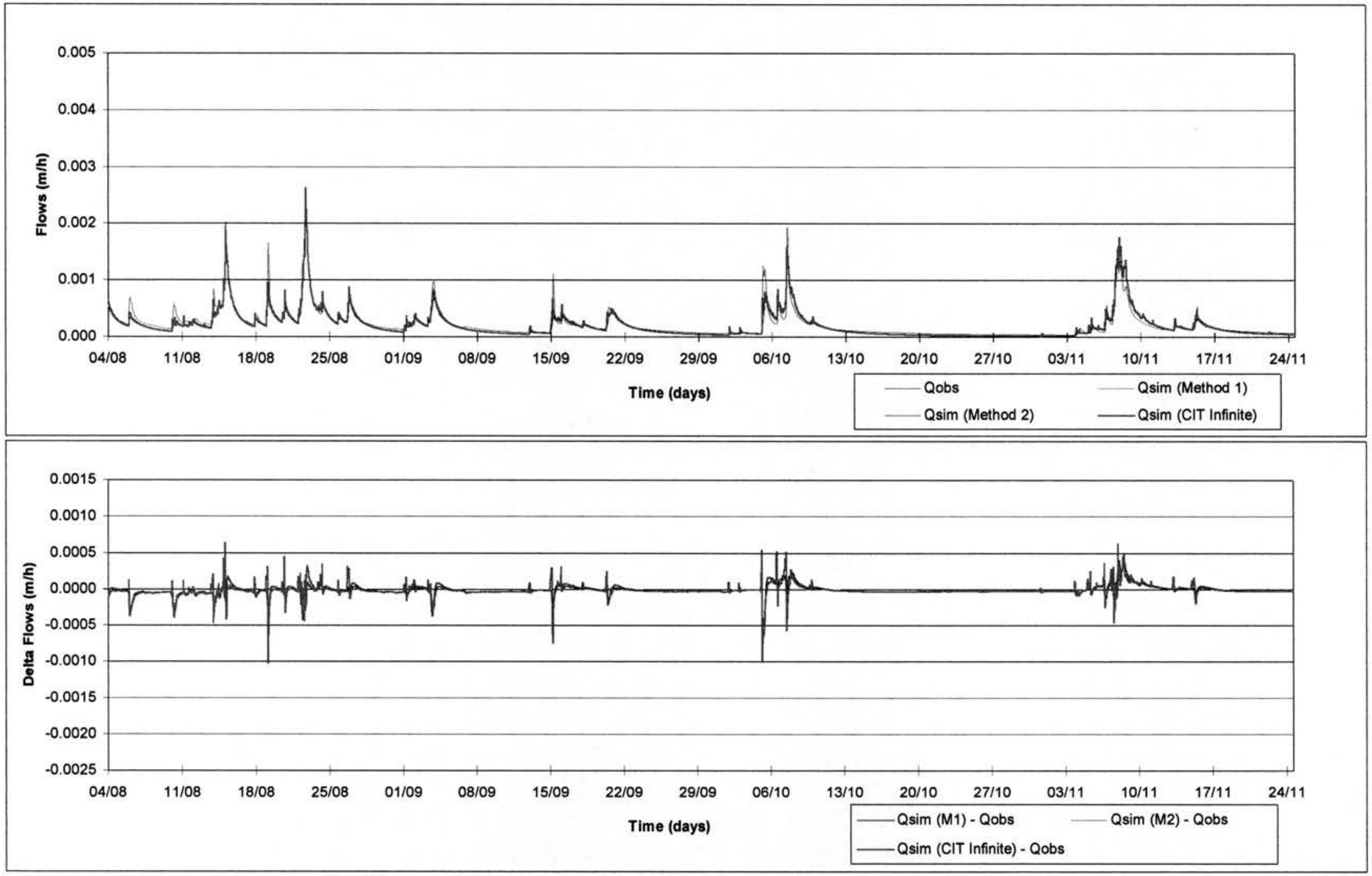


Figure 4.17b - Hydrographs obtained with CIT Methods - Hafren 1985

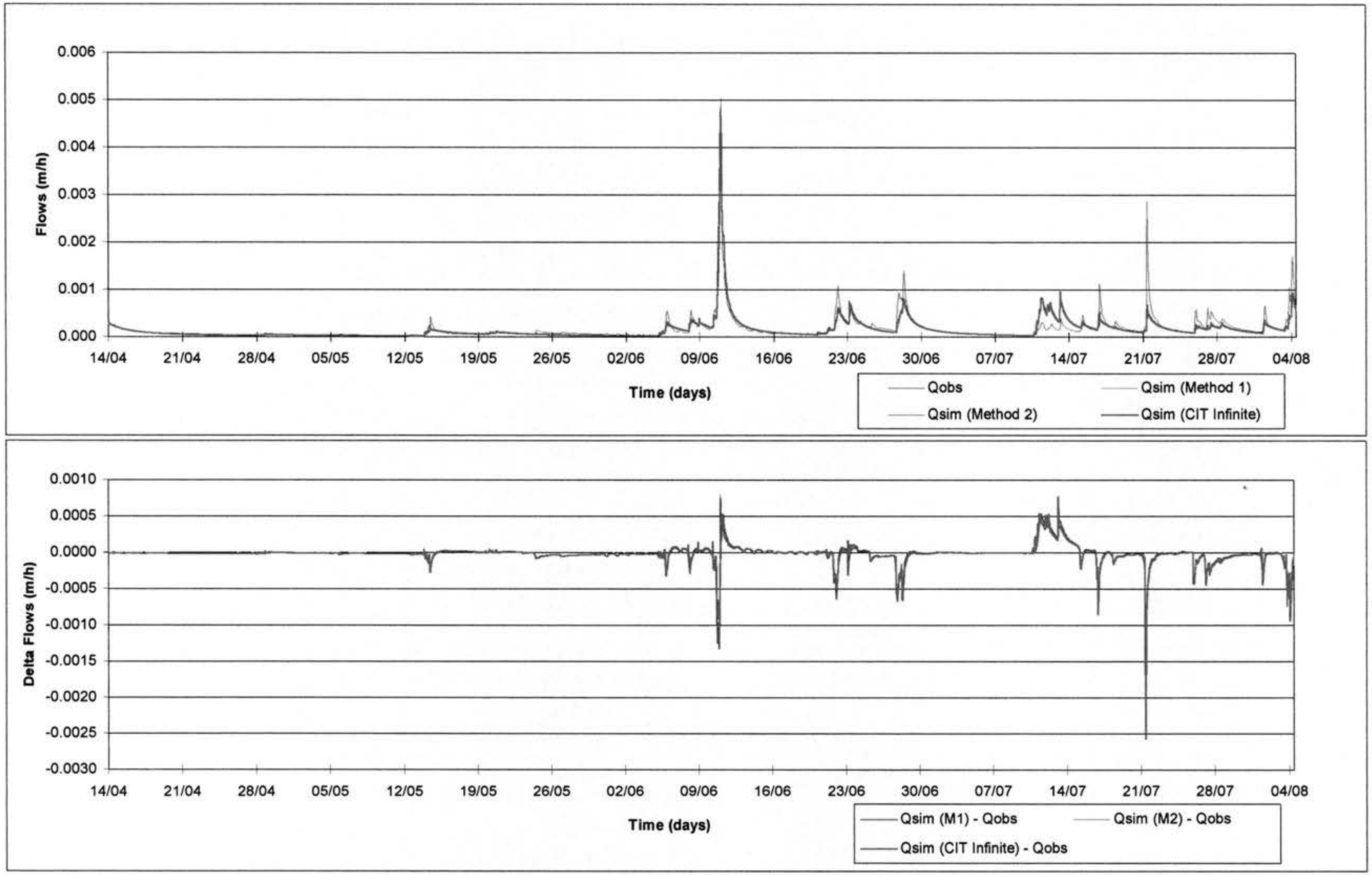


Figure 4.18a - Hydrographs obtained with CIT Methods - Upper Hore 1985

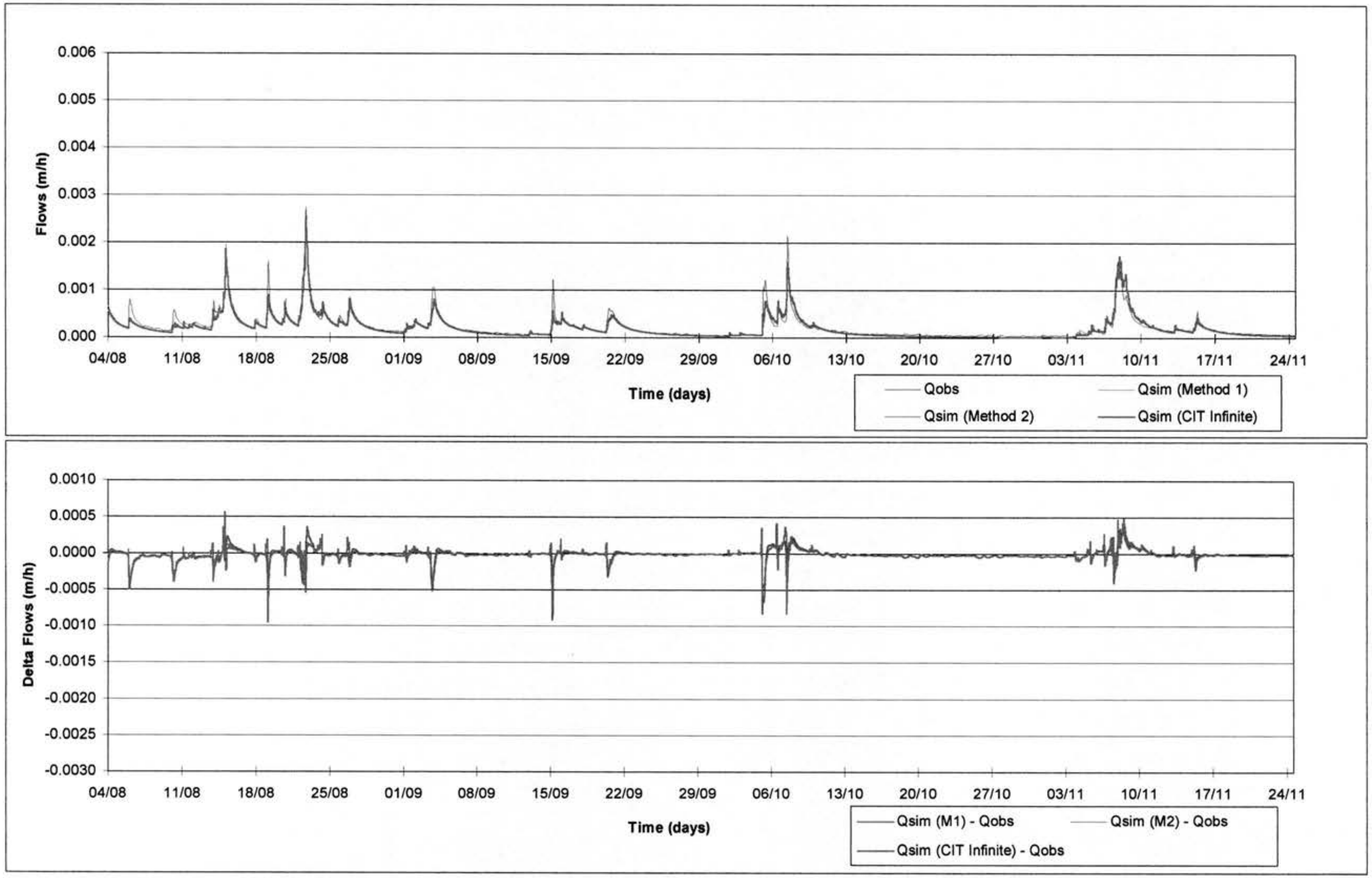


Figure 4.18b - Hydrographs obtained with CIT Methods - Upper Hore 1985

4.6 Simulations of Single Flood Events

Having identified the spatial distribution of K_0 that gave the best catchment and subcatchment outflow efficiencies the next step involved selecting single flood events during the 1985 simulation period, and comparing the results for constant K_0 and HOST-SPR K_0. The four events selected for analysis are summarised in Tab. 4.15 and simulations were carried out both for the Hafren and for the Upper Hore.

	Start (hrs)	Start (date)	End (hrs)	End (date)	Hafren Observed Flow (m/h)	Upper Hore Obs. Flow (m/h)
Event 1	3854	9/6/85	4099	19/6/85	0.00017902	0.000193
Event 2	4307	28/6/85	4776	18/7/85	0.00096695	0.0009921
Event 3	4803	19/7/85	4962	25/7/85	0.00020025	0.00020559
Event 4	5476	16/8/85	5865	1/9/85	0.00058419	0.00054729

Table 4.15 - Periods of Single Event Simulations 1985

The events represent a mixture of single peak and multi-peak floods chosen over the late spring and summer months of the simulation period, when it is expected that there should be a wide range of variation in soil moisture deficit due to the higher temperatures and evapotranspiration rates. From an examination of the potential ET data, maximum values of 0.010 - 0.013 m/d are observed in this period, compared to values less than 0.004 m/d in the winter months.

Furthermore, the events include three of the highest flood peaks of 1985, which it is expected will be associated with the largest extent of saturated areas. It should also be noted that all the simulation intervals have been chosen so as to include the recession limb of the preceding event. This has been done to allow for an adequate period of initialisation of the water storages in TOPMODEL.

4.6.1 Hafren Event Simulations

The chosen events are indicated in Fig. 4.11 and we can note in particular that:

- Event 1 is a single peak flood event occurring in mid-June with the highest yearly observed flow (approx. 0.004 m/h) and a good visual match between Qsim and Qobs;
- Event 2 is a multi-peak flood event starting at the end of June with a significant overestimation of Qsim compared to Qobs;
- Event 3 is a single peak flood occurring in late July which presents a good visual match between Qsim and Qobs except for a significant underestimation of the simulated floodpeak;
- Event 4 is a multi-peak flood occurring in late August which presents a good overall match between Qsim and Qobs.

In comparison to the full year simulation results, the analysis of individual events provides more detailed information on TOPMODEL's performance. Considering the summary of the separate events in Tab. 4.16 and the event hydrographs, a brief analysis is presented in the following paragraphs.

HAFREN 1985	EVENT 1 (3854-4099)		EVENT 2 (4307-4776)		EVENT 3 (4803-4962)		EVENT 4 (5476-5865)	
Soil Distribution	***Const. K0***	***HOST SPR***	***Const. K0***	***HOST SPR***	***Const. K0***	***HOST SPR***	***Const. K0***	***HOST SPR***
TOPMODEL Parameters								
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	n.a.	890.978	n.a.	890.978	n.a.	890.978	n.a.
T0=m*KO (m^2/h)	11.761	11.761	11.761	11.761	11.761	11.761	11.761	11.761
Spatially Avg. K0	n.a.	890.981	n.a.	890.981	n.a.	890.981	n.a.	890.981
Gamma	5.212	5.328	5.212	5.328	5.212	5.328	5.212	5.328
EFFICIENCY '85	**97.41%**	**97.50%**	**-52.65%**	**-53.39%**	**54.61%**	**55.91%**	**91.38%**	**90.86%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW								
SAT. ZONE RECHARGE (m)	0.066	0.066	0.082	0.081	0.022	0.022	0.113	0.112
BASEFLOW (m)	.080 / 93.75	.080 / 93.20	.102 / 135.16	.101 / 134.25	.031 / 77.56	.031 / 77.13	.138 / 88.93	.137 / 88.31
SAT. EXCESS FLOW (m)	.011 / 13.40	.012 / 13.65	.006 / 8.17	.007 / 9.24	.002 / 3.88	.002 / 4.24	.012 / 7.48	.013 / 8.13
SAT. FROM ABOVE (m)	.001 / 1.24	.001 / 1.54	.000 / .53	.000 / .49	.000 / .23	.000 / .39	.001 / .39	.001 / .39
WATER BALANCE								
TOTAL SIMULATED FLOWS (m)	0.093	0.093	0.109	0.109	0.032	0.032	0.150	0.150
TOTAL OBSERVED FLOWS (m)	0.086	0.086	0.075	0.075	0.040	0.040	0.155	0.155
TOTAL RAINFALL (m)	0.089	0.089	0.128	0.128	0.031	0.031	0.173	0.173
TOTAL POTENTIAL ET (m)	0.073	0.073	0.158	0.158	0.043	0.043	0.062	0.062
TOTAL PREDICTED ET (m)	0.016	0.016	0.048	0.048	0.014	0.014	0.048	0.048
FINAL BUDGET	-0.013	-0.013	-0.018	-0.018	-0.011	-0.011	0.000	0.000

Table 4.16 - Summary of Hafren Event Simulations

- In event 1 (Fig. 4.19) the very high efficiencies (97.50%) are associated with baseflow component percentages of 93-94%, which are higher than the full year simulation values (89-90%). The saturation flow components are also higher than the full year results (~14% vs. ~8%). There is a very good match to increasing flood flows as well as to the recession limb of the hydrograph, but there are noticeable errors in the simulated flow at the beginning of the event, at the flood peak and early in the recession limb.

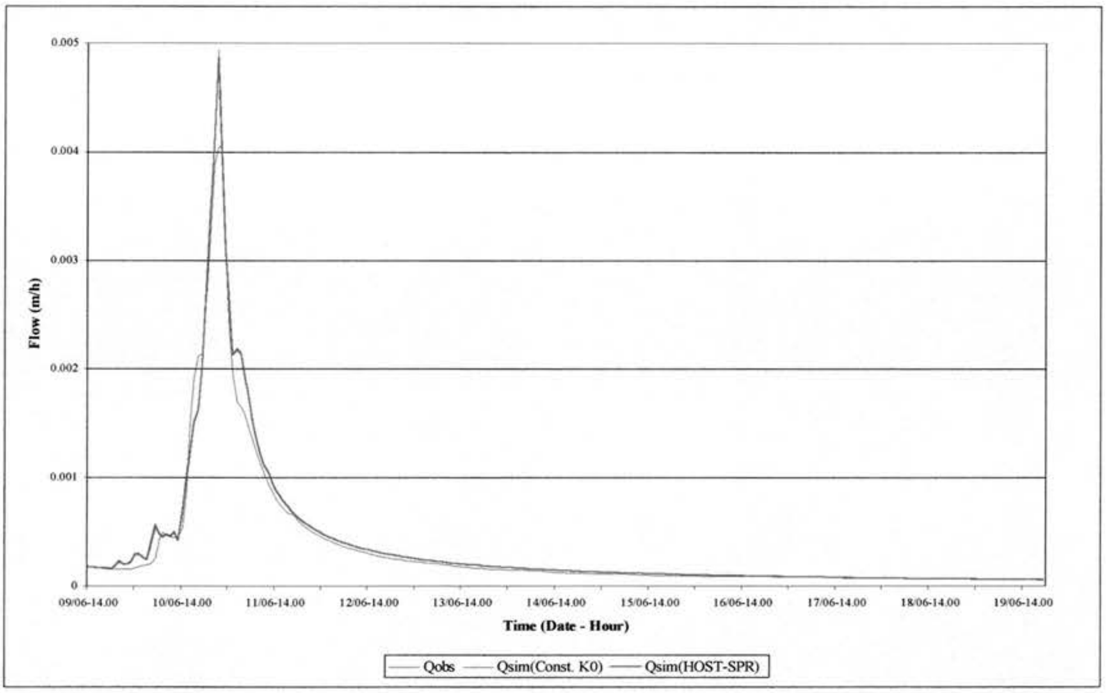


Figure 4.19 – Hafren Hydrographs for Event 1

- In event 2 (Fig. 4.20) the low efficiencies (-53%)[9] are associated with values of baseflow component which are significantly higher than those found for the entire year (~135% vs. 89%). The saturation flow components are instead similar to those found for the entire simulation period (9-10%). Even though the preceding recession limb is matched very well, the first four flood peaks (11/7-13/7) are grossly overestimated by the model, though the time to concentration of the main flood peaks is accurately predicted. The match on the fifth flood peak (15/7) is quite good while on the last flood peak (16/7) the simulated flow is underestimated. For both of the last two flood events, it is also apparent that the slope of the recession limb of the hydrographs is not matched very well.

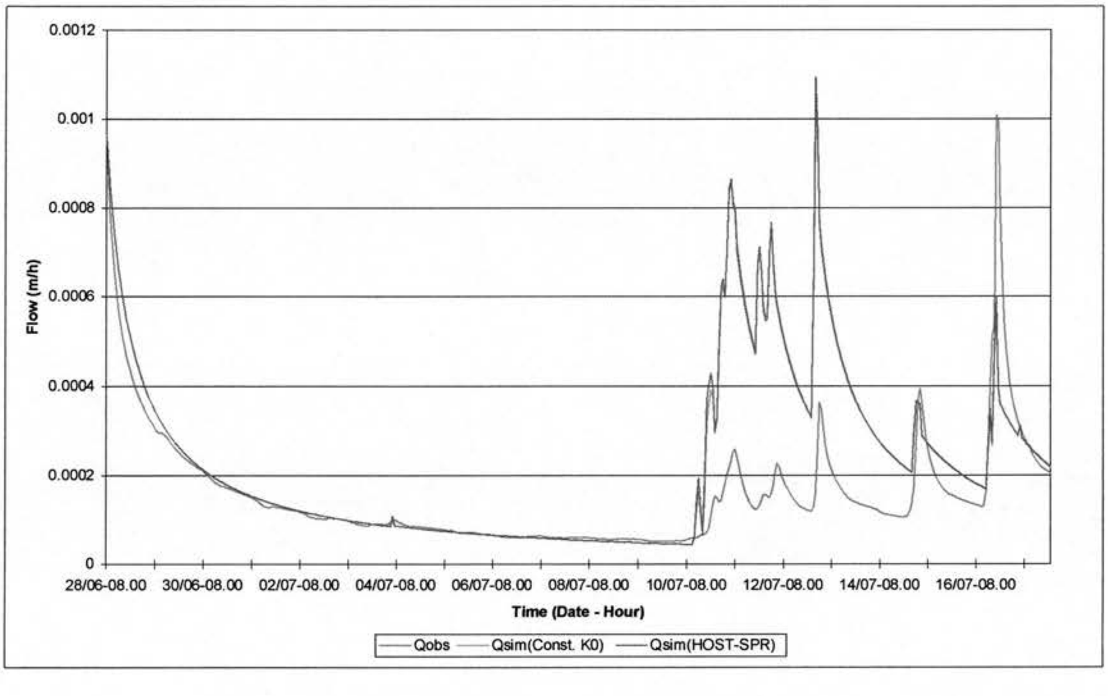


Figure 4.20 - Hafren Hydrographs for Event 2

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[9] It should be remembered that a negative efficiency simply implies that over the period considered the variance of the residual error is greater than that of the observed flows. The efficiency criterion has previously been described in Section 3.3.7

* In event 3 (Fig. 4.21) the low efficiencies (~55%) are associated with values of baseflow component and saturated flow components which are both significantly lower than those found for the entire 1985 simulation period. In particular, the baseflow component is ~77% while the saturated flow components are ~ 4% of total observed flows. Even though the recession limbs preceding and following the flood peak are matched very well, there is a marked underestimation of the flood peak.

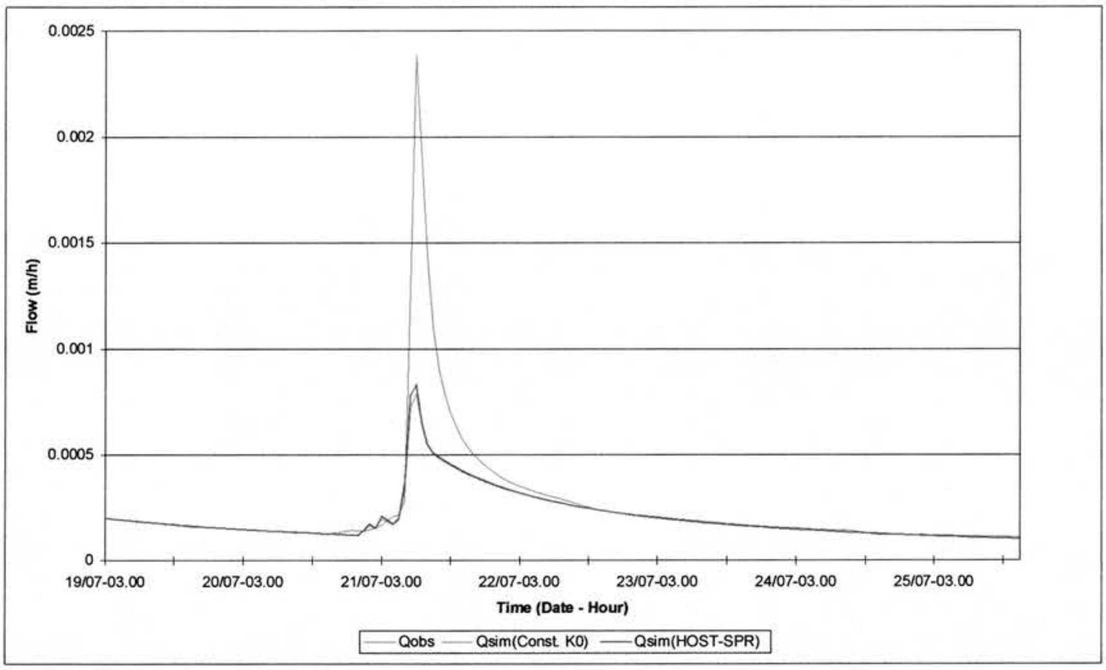

Figure 4.21 - Hafren Hydrographs for Event 3

- In event 4 (Fig. 4.22) the high efficiencies (91%) are associated with values of baseflow and saturated flow components - ~89% and ~8% respectively - which are similar to those found for the entire 1985 simulation period. From an examination of the hydrographs we can see that even though the first flood peak (19/8) is underestimated, the rest of the event is simulated exceptionally well by the model. This is further confirmed by the closeness in the values of total simulated flows and total observed flows, as well as by the final balance value of zero in Tab. 4.16.

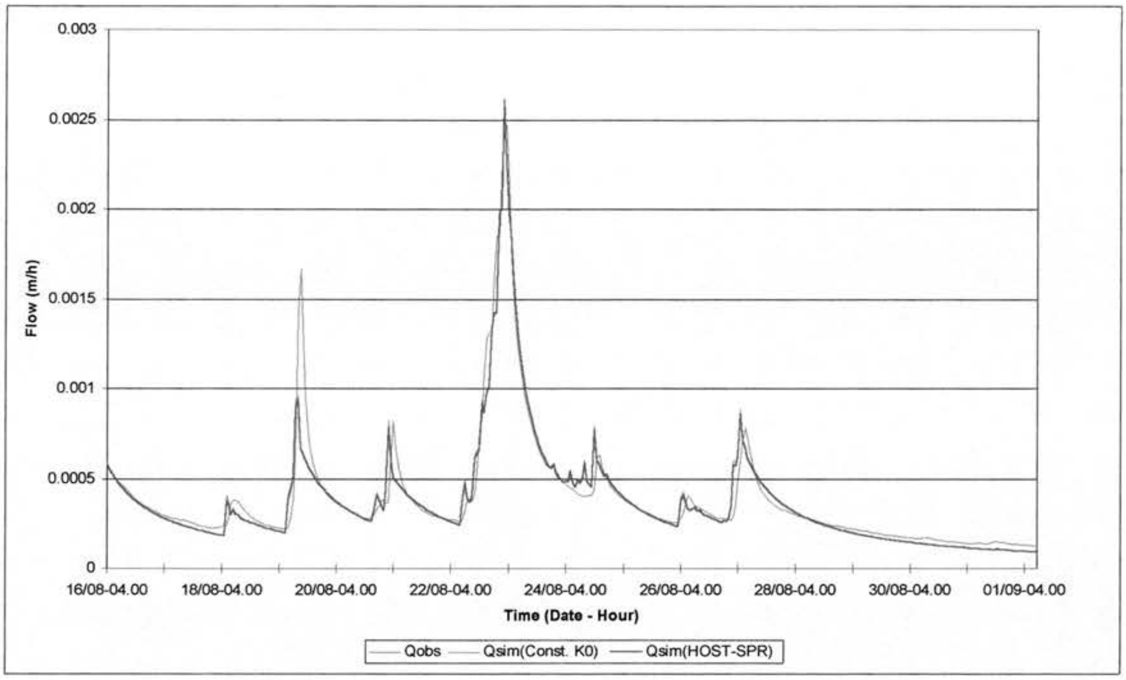

Figure 4.22 - Hafren Hydrographs for Event 4

4.6.2 Upper Hore Event Simulations

Before analysing the single events, it should be noted that the single event simulations for the Upper Hore were carried out only for the HOST-SPR K_0 because:

a) the full year simulations had already confirmed the similarity between constant K_0 and HOST-SPR hydrographs, for both the Hafren and the Upper Hore;
b) it was thought useful to verify whether there were any noticeable differences in the HOST-SPR hydrographs, compared to the Hafren simulations.

The four events present very similar characteristics to the corresponding events in the Hafren:

- Event 1 is a single peak flood event occurring in mid-June with the highest yearly observed flow (approx. 0.005 m/h) and a good visual match between Qsim and Qobs;
- Event 2 is a multi-peak flood event starting at the end of June with a significant overestimation of Qsim with respect to Qobs;
- Event 3 is a single peak flood occurring in late July which presents a good visual match between Qsim and Qobs except for a significant underestimation of the simulated floodpeak;
- Event 4 is a multi-peak flood occurring in late August which presents a good overall match between Qsim and Qobs.

A summary of the simulations for the four events is given in Tab. 4.17, while the individual event hydrographs are shown in Figs. 4.23, 4.24, 4.25, 4.26. The plots of the Upper Hore hydrographs clearly confirm that even within single events, there appear to be no significant differences compared to the Hafren HOST-SPR hydrographs. The significance of these similarities will be discussed in the following chapter.

UPPER HORE 1985 ***Soil Distribution***	**EVENT 1 (3854-4099)** ***HOST SPR***	**EVENT 2 (4307-4776)** ***HOST SPR***	**EVENT 3 (4803-4962)** ***HOST SPR***	**EVENT 4 (5476-5865)** ***HOST SPR***
TOPMODEL Parameters				
m (m)	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	n.a.	n.a.	n.a.	n.a.
T0=m*K0 (m^2/h)	11.7609	11.7609	11.7609	11.7609
Spatially Avg. K0 (m)	890.9764	890.9764	890.9764	890.9764
Gamma	4.985	4.985	4.985	4.985
EFFICIENCY '85	**95.98%**	**-6.89%**	**45.72%**	**91.81%**
EFFICIENCY HAFREN '85	97.50%	-53.39%	55.91%	90.86%
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW				
SAT. ZONE RECHARGE (m)	0.068	0.083	0.022	0.115
BASEFLOW (m)	.083 / 94.27	.103 / 130.18	.031 / 74.38	.138 / 89.51
SAT. EXCESS FLOW (m)	.009 / 10.72	.005 / 6.61	.001 / 3.18	.010 / 6.54
SAT. FROM ABOVE (m)	.001 / 1.20	.000 / .46	.000 / .20	.000 / .30
WATER BALANCE				
TOTAL SIMULATED FLOWS (m)	0.094	0.109	0.033	0.149
TOTAL OBSERVED FLOWS (m)	0.088	0.079	0.042	0.155
TOTAL RAINFALL (m)	0.089	0.128	0.031	0.173
TOTAL POTENTIAL ET (m)	0.073	0.158	0.043	0.062
TOTAL PREDICTED ET (m)	0.016	0.048	0.014	0.048
FINAL BUDGET	-0.013	-0.018	-0.011	0.000

Table 4.17 - Summary of Upper Hore Event Simulations

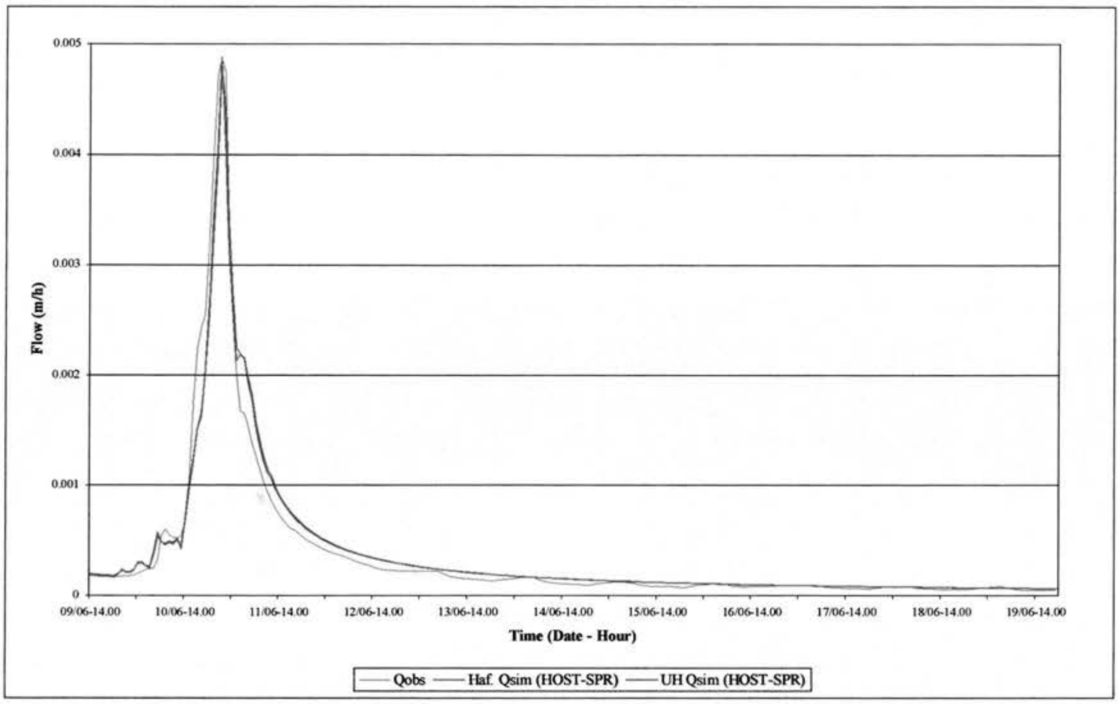

Figure 4.23 – Upper Hore Hydrographs for Event 1

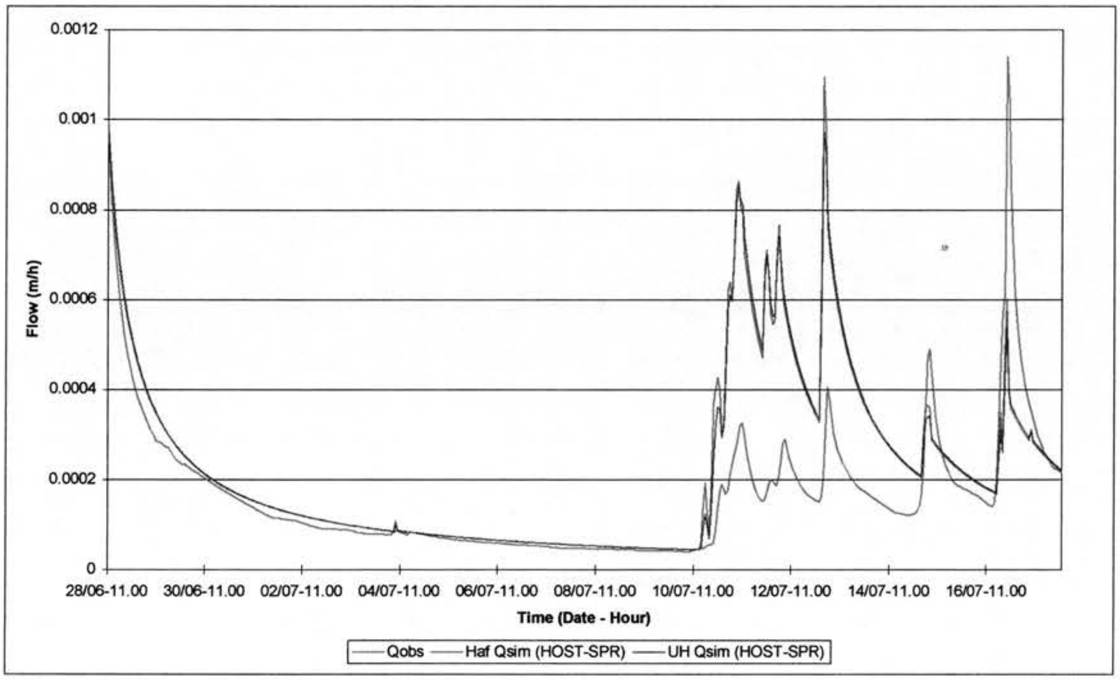

Figure 4.24 - Upper Hore Hydrographs for Event 2

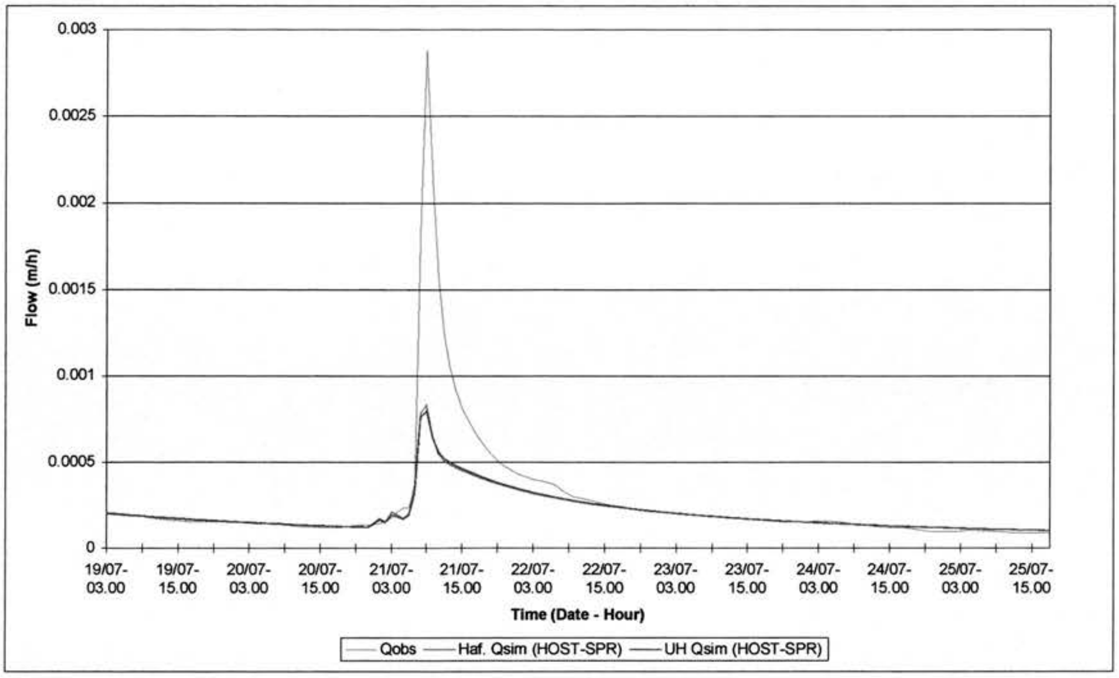

Figure 4.25 - Upper Hore Hydrographs for Event 3

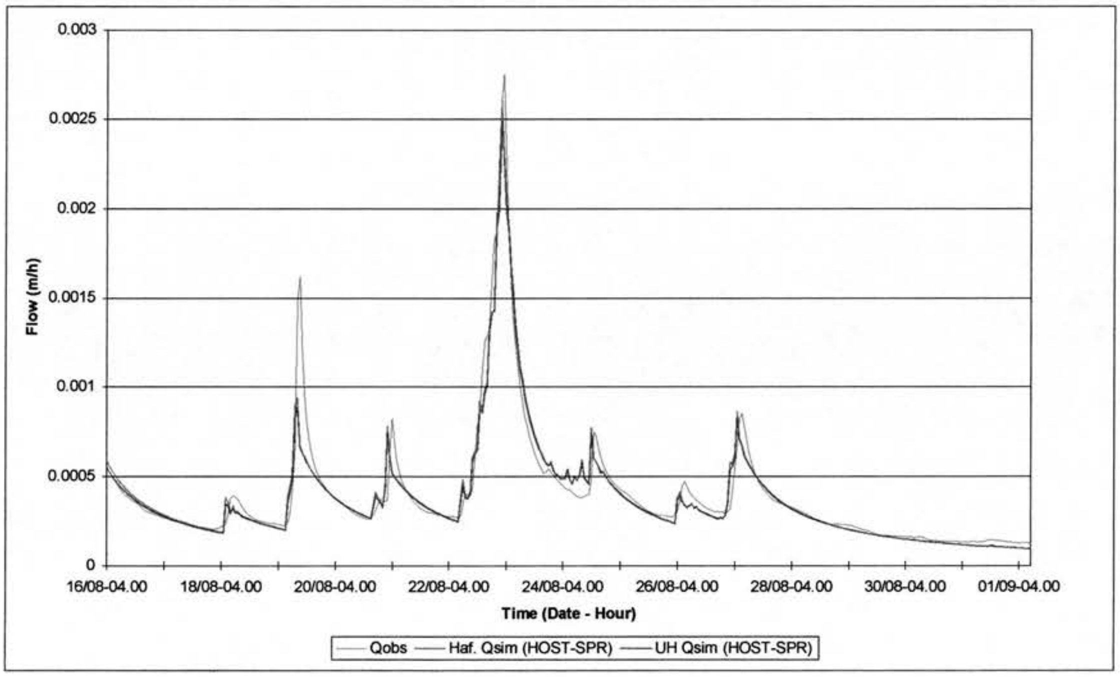

Figure 4.26 - Upper Hore Hydrographs for Event 4

4.7 Determination of Spatially Distributed Soil Moisture Deficits

The predicted outflow hydrographs for the single events showed that there was no significant variation from the constant K_0 case with the inclusion of spatially variable K_0 values. The only remaining aspect to consider therefore was the prediction of spatially distributed soil moisture deficits (SMD).

For the four flood events already selected, the spatio-temporal patterns of soil moisture deficit (SMD) were determined only for the Hafren catchment. This would allow us to identify the spatial distribution and extent of soil moisture deficit and saturated runoff generating areas and verify whether there was any dependence between soil variability and model performance. The SMD calculations were not carried out for the Upper Hore because the almost identical event hydrographs in Section 4.6 confirmed that TOPMODEL predictions were not affected by catchment scale.

Within each of the selected events, a discrete number of timesteps were selected, mainly corresponding to one of the following conditions:

a) the beginning of the flood event;

b) the maximum flood peak during the event;

c) any intermediate peaks and troughs in the flood hydrograph;

d) drainage phase (after rainfall event) associated with hydrograph recession limb.

This made it possible to not only examine the soil moisture distribution at extreme conditions, but also at intermediate conditions within the single events. A summary of the chosen timesteps, together with the catchment average SMD values calculated by TOPMODEL for the HOST-SPR distribution is given in Tab. 4.18.

For each of the selected time steps, the soil moisture deficit data produced by TOPMODEL was imported into ArcView where the data could be more effectively represented as thematic maps, and these have all been included in Appendix 2.

Event ID	Timestep (hrs - date)	Hafren Avg. SBAR (m)	Description of Hydrograph Point
E1-T1	3877 - 10/6	$3.36*10^{-2}$	Beginning of rising limb of hydrograph
E1-T2	3887 - 10/6	$5.31*10^{-3}$	Maximum flood peak for 1985
E1-T3	4099 - 19/6	$5.76*10^{-2}$	Last point on hydrograph recession.
E2-T1	4598 - 10/7	$6.25*10^{-2}$	Beginning of rising limb of hydrograph
E2-T2	4617 - 11/7	$2.60*10^{-2}$	Intermediate flood peak.
E2-T3	4657 - 13/7	$3.59*10^{-2}$	Intermediate flood minimum
E2-T4	4659 - 13/7	$2.72*10^{-2}$	Maximum flood peak.
E2-T5	4744 - 14/7	$4.45*10^{-2}$	Intermediate flood minimum
E2-T6	4749 - 16/7	$3.44*10^{-2}$	Intermediate flood peak
E3-T1	4847 - 20/7	$5.08*10^{-2}$	Beginning of rising limb of hydrograph
E3-T2	4858 - 21/7	$3.12*10^{-2}$	Maximum flood peak
E3-T3	4890 - 22/7	$4.09*10^{-2}$	Intermediate point on hydrograph recession.
E4-T1	5551 - 19/8	$4.23*10^{-2}$	Beginning of rising limb of hydrograph
E4-T2	5556 - 19/8	$2.63*10^{-2}$	Intermediate flood peak.
E4-T3	5642 - 23/8	$1.18*10^{-2}$	Maximum flood peak
E4-T4	5650 - 24/8	$2.09*10^{-2}$	Intermediate point on hydrograph recession

Table 4.18 – Timesteps of Soil Moisture Deficit Simulations

From a visual examination of the maps, a dominant trend appears immediately. This regards the pattern with which the saturated runoff generating areas expand. Starting off from the riparian areas adjacent to the drainage network, the saturated areas expand upslope and only in the proximity of the flood peak do the blanket peats in the upper reaches of the catchment become extensively saturated. Conversely, in the drainage phase the blanket peats drain relatively quickly, and then the hillslopes become progressively drier until the saturated areas once again coincide with the riparian areas. This trend will be examined further in the following chapter, supported by a selection of the SMD maps.

4.7.1 Quantitative Analysis of SMD Maps

The SMD maps produced are useful for the visual identification and comparison of saturation patterns in the catchment, and to assess the degree to which predicted saturation follows patterns expected from field-based knowledge. Yet it is difficult for an observer to identify and extract quantifiable differences between the various K_0 distributions, especially if multiple timesteps need to be considered. In order to better comprehend the significance of the information contained within the saturation deficit maps, it was decided to carry out a quantitative comparison of the SMD maps. In particular, we were interested in identifying any systematic variations between the SMD predictions obtained with the constant K_0 and the variable HOST SPR K_0 distributions.

The procedure adopted involved the following steps.

a) For each of the four events chosen for the Hafren the SMD maps obtained for constant K_0 were subtracted from those of HOST-SPR K_0 at each timestep. This provided a cell-by-cell measure of the SMD difference between estimated SMD in the two cases. This result was also mapped for each of the timesteps in Table 2.18 so that any correlation between topography, soils and SMD variations could be visually identified (Appendix 3).
b) From the cell values the catchment total SMD difference and the average difference associated with each soil class were calculated. This allowed us to evaluate a total catchment measure of variation, as well as identifying the contributions of the six soil classes to the total SMD difference.
c) The calculations were repeated for every timestep in each of the chosen events, thus obtaining the variation of the total and soil class SMD differences over time.

The above three steps are summarised in the following equations (Eqn. 4.2 - 4.5).

$$\Delta SMD(x,y,t) = SMD(x,y,t)_{HOSTK0} - SMD(x,y,t)_{Const.K0} \qquad \text{Eqn. 4.2}$$

$$\Delta SMD(t) = \sum_{x,y} \Delta SMD(x,y,t) \qquad \text{Eqn. 4.3}$$

$$\Delta SMD(soil,t) = SMD(soil,t)_{HOSTK0} - SMD(soil,t)_{Const.K0} \qquad \text{Eqn. 4.4}$$

$$avg\Delta SMD_{soil}(t) = \frac{\sum_{soil} \Delta SMD(soil,t)}{\sum tot.areabysoilclass} \qquad \text{Eqn. 4.5}$$

The results associated with equations 4.3 and 4.5 were plotted as a function of time for the four flood events (Figs. 4.27, 4.28, 4.29, 4.30). Given the absence of field measured SMD data against which to compare the differences, plots of Qsim and Qobs are also shown.

When examining the plots, the reader should bear in mind that the total SMD difference does not necessarily reflect variations in the average SMD difference by soil type. This is due to the prevalence of the Crowdy, Skiddaw and Wilcock soils within the catchment. As a result, even small variations in the average soil SMD difference of the above soils can have a significant impact on the total SMD difference for the catchment. For example, during the period 9/6 to 10/6 in event 1, the Hafren soils show a much smaller increase in the SMD difference by soil type, than the Aled and Manod soils. But because the Hafren soils occupy such a large portion of the catchment, the overall effect is a significant increase in the total catchment SMD difference. Conversely, between 10/6 and 11/6 the very slight decrease in the SMD difference of the Crowdy, Skiddaw and Wilcock soils determines a drastic drop in the total catchment SMD difference.

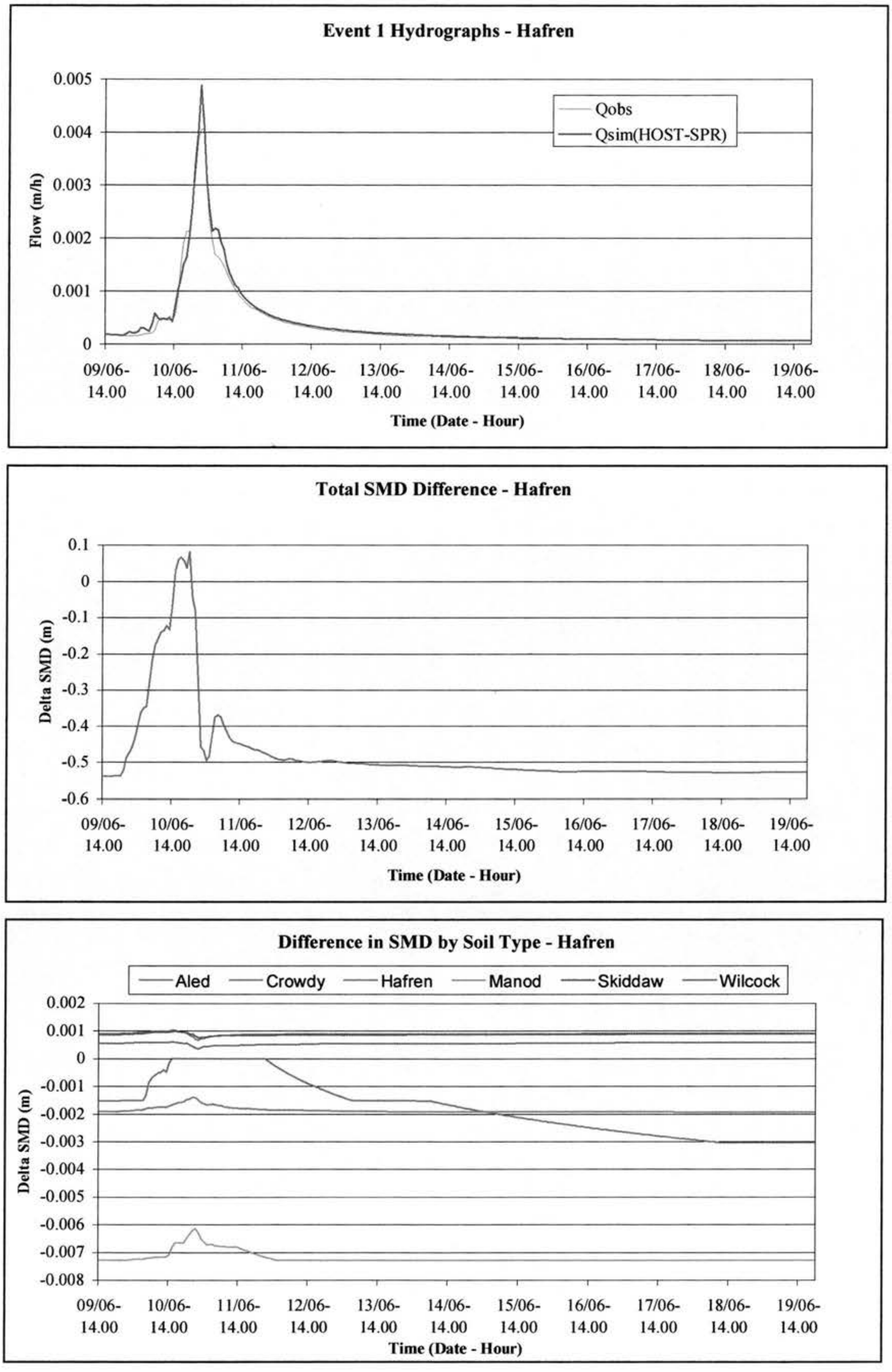

Figure 4.27 - Event 1 SMD Calculations

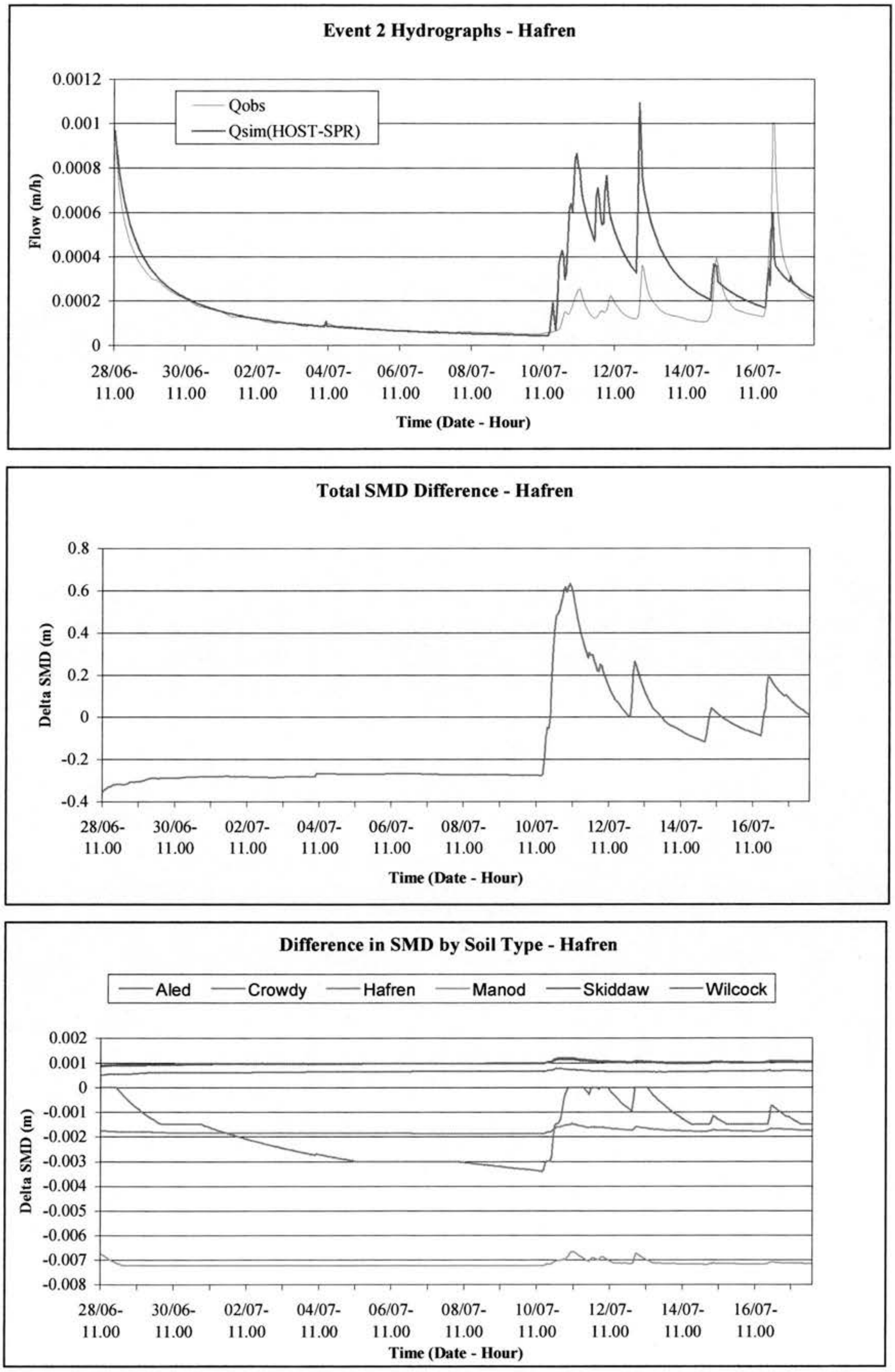

Figure 4.28 - Event 2 SMD Calculations

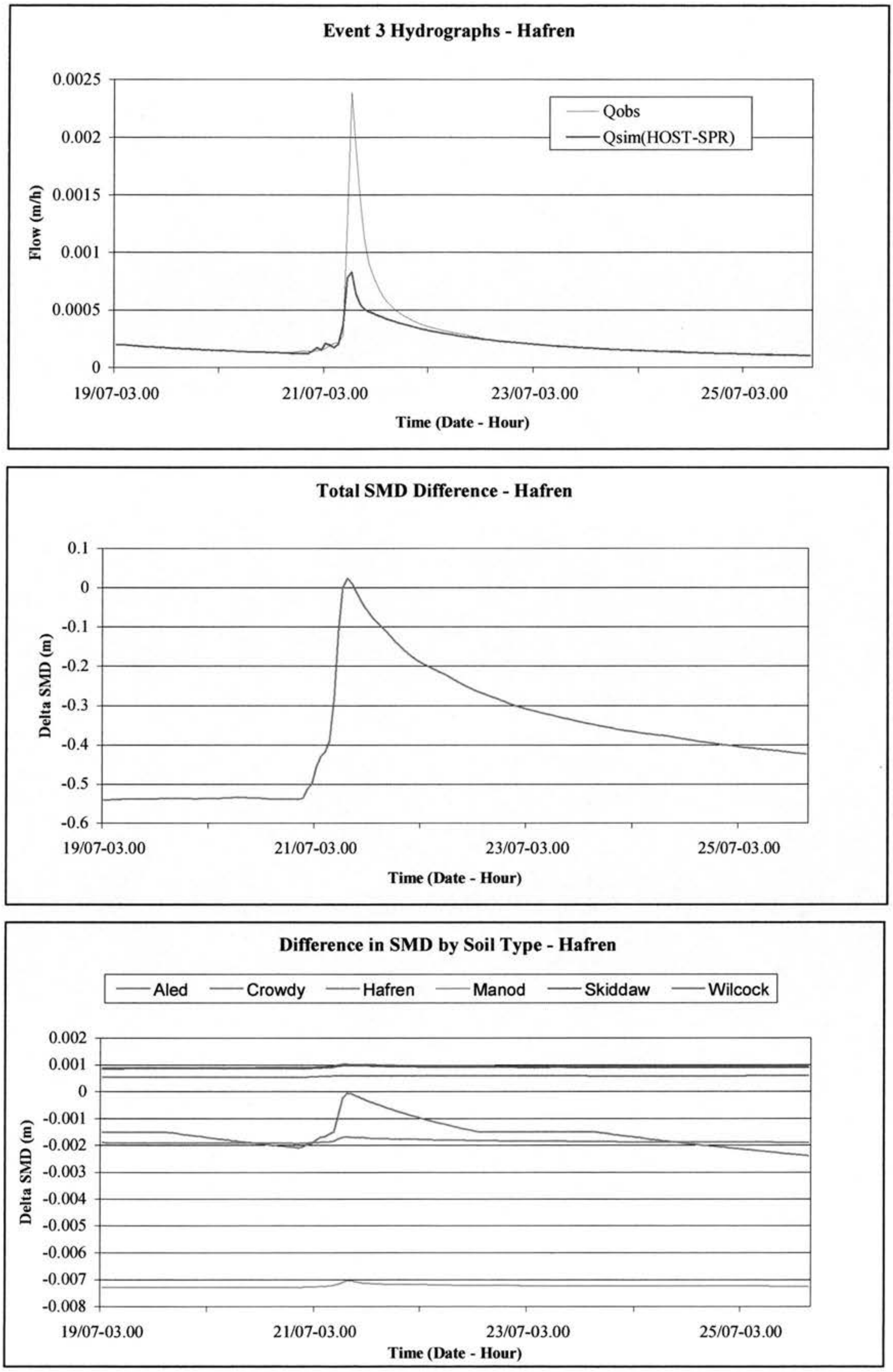

Figure 4.29 - Event 3 SMD Calculations

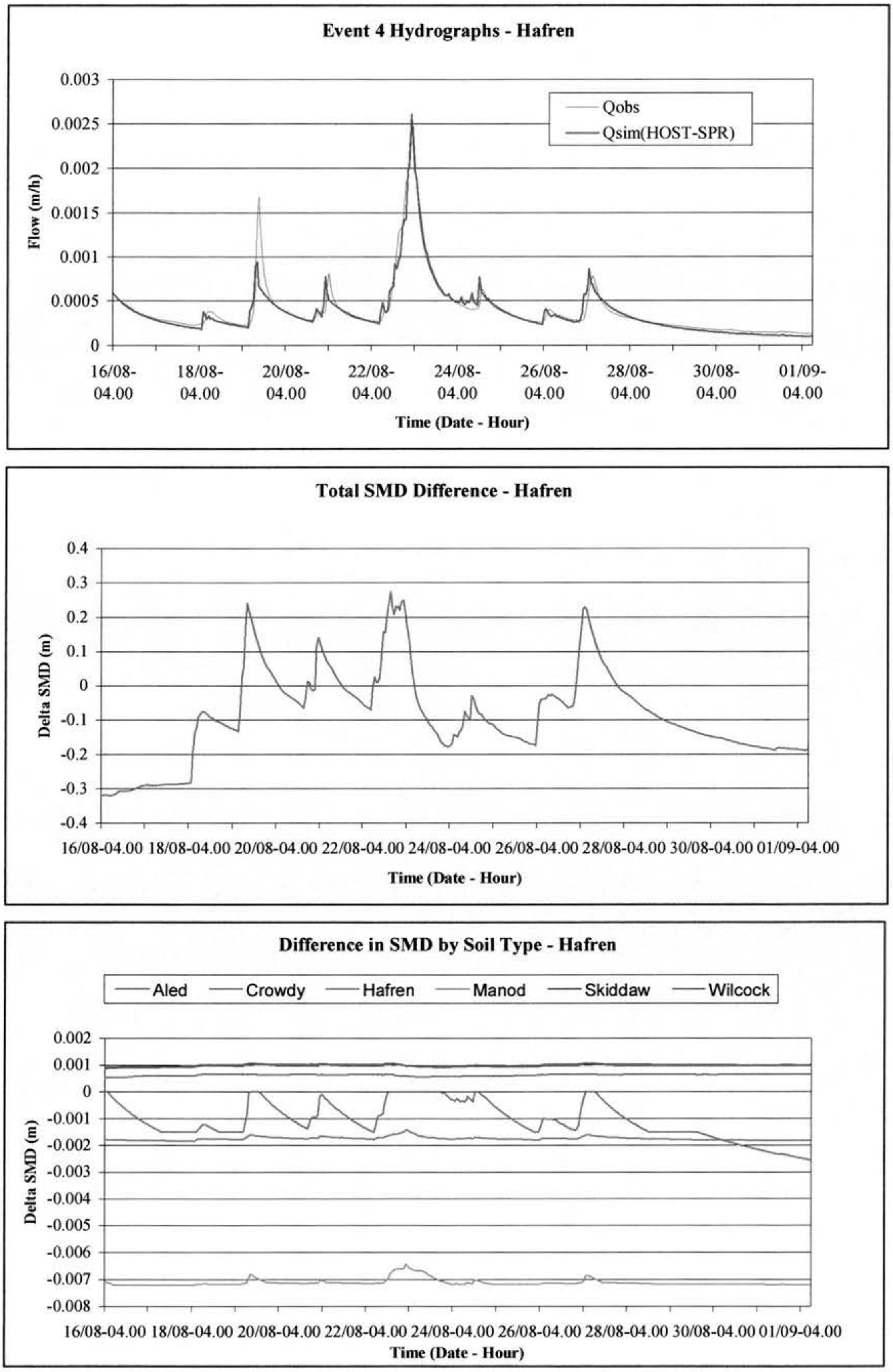

Figure 4.30 - Event 4 SMD Calculations

From an examination of the plots, several observations can be made.

1) For all of the events the total SMD difference shows negative values except in the vicinity of observed flood peaks.
2) For events 2, 3 and 4 the total SMD difference curves present peaks which slightly anticipate the observed flow peaks by 1-2 hours.
3) For all events the soils which show the greatest variation in SMD differences over time are the Aled and Manod soils. For both soils the differences are always less than or equal to zero, and the timing of the flood peaks essentially reflects the timing of the peaks in total SMD difference.
4) Over all four events the differences in SMD are essentially constant for the Crowdy, Hafren, Skiddaw and Wilcock soils.

The significance of these results, in relation to TOPMODEL's ability to predict spatially distributed soil moisture deficit and runoff, will be examined in the following chapter.

4.8 Conclusions

The results presented in this chapter have provided a description of all the principal findings obtained with the TOPMODEL simulations. Following the procedure set out in Section 3.9 the principal aim was to identify the effects of a spatially variable K_0 on the performance of TOPMODEL:

a) in terms of total catchment or subcatchment outflow over a hydrological year (excluding the snow months);
b) in terms of prediction of total outflow for single flood events;
c) in terms of the ability to predict soil moisture deficit (SMD) and saturated runoff generating areas.

Based on the findings illustrated in this chapter it does not appear that the introduction of a spatially variable K_0 has had the marked effect that was anticipated. An analysis of the possible reasons for this will be presented in the following chapter.

5. Interpretation of Simulation Results

The present chapter will analyse and interpret the significance of the simulation results presented in the preceding chapter. It will begin by evaluating the preprocessing of the input data and identifying any problems that affected the subsequent simulations. Then it will go on to examine the issue of model performance, measured in terms of total catchment outflow, and how this was affected by the introduction of a spatially variable K_0. More importantly, it will consider the maps of predicted soil moisture deficit and evaluate whether incorporating spatially variable K_0 values has resulted in a more realistic representation of spatially distributed soil moisture deficit values. Finally, the methods and results of the present research will be assessed in relation to the wider context of TOPMODEL research and, more generally, distributed catchment modelling.

5.1 Preprocessing of Input Data

The preparation of input GIS coverages from the topographic and soil maps was a relatively simple, though lengthy, procedure. Once the contour and spot heights were digitised, a continuous gridded DEM was generated using the Inverse Distance Weighting (IDW) interpolation method in ARC-INFO GRID. In terms of possible sources of error, two factors may have lead to interpolation errors.

a) The digitised coverage contained both contours and spot heights, and it is the latter which are generally considered to be the more accurate values. The IDW algorithm though does not allow the assignment of weights to the different types of values and this may have led to errors in the interpolated DEM. This may be especially true at the higher grid resolutions where the sparsity of spot heights within cells is greater.

b) At the higher resolution there may be DEM cells without any digitised points in the surrounding 3*3 window. In such cases the IDW algorithm will use points from cells within a pre-specified search radius. If there are insufficient points, then the interpolated elevations will be of poorer accuracy.

Given that the present research was more concerned with the hydrological application of the DEM, a topographic validation of the interpolated DEM was not carried out. The DEM was instead validated in relation to the existence of sinks within the catchment. Sinks may not necessarily represent actual elevation errors, but in terms of the calculation of hydrological drainage flow paths they represent inconsistent values which need to be corrected.

In order to be able to evaluate the extent of the problem TOPMODEL's *sink.for* module was used to determine the number of sinks in each of the 10m, 25m and 50m DEMs and these are shown in Tab. 5.1. It is apparent that as the DEM resolution increases so does the number of sinks. This could in part be due to the combined effect of the two factors discussed above, or it could reflect a greater accuracy in the prediction of topographic hollows within the catchment. In either case though, the sinks must be filled to ensure the hydrological consistency of the DEM, even at the expense of topographic accuracy.

	50m DEM	**25m DEM**	**10m DEM**
No. of Sinks Found	2	201	12434
Max. Sink Depth	1.04m[1]	8.87m	4.11m
Max. Sink Coordinates (x,y)[2]	(30, 11)	(74, 74)	(276, 310)
DEM size (rows x cols)	(76 x 82)	(152 x 164)	(380 x 410)
Note 1: For the 50m DEM the max. depth was equal to the manual correction applied to ensure sink-filling and hydrological consistency. **Note 2:** The relative coordinates are given as (nrow,ncol) because these were used in the TOPMODEL input files.			

Table 5.1 – Summary of Sinks found in Interpolated DEMs

While the sinks could all have been automatically filled using *sink.for* - or ARC-INFO GRID - this option was not pursued because it could have led to significant, and uncontrollable, changes being made to the DEM. As shown in the work done by Hutchison (1988, 1989) uncritical enforcement of sink-filling in DEMs could lead to unrealistic changes in elevations and slope, which compromise hydrological consistency in the corrected DEM. Within the general context of hybrid index-based models, changes in slope and drainage paths would in turn affect the prediction of the wetness index distribution and, consequently, the predicted runoff source areas. Especially in very small upland catchments such as the Hafren, this could lead to significant impacts on catchment outflow prediction, as well as on the estimation of internal catchment conditions (eg. soil moisture deficit).

For each of the three DEMs (10m, 25m, 50m) the topographic index curves were calculated before and after sink-filling, in order to identify any differences. The 50m DEM was finally chosen for the model simulations because:

a) of the three DEMs it showed the least difference in the topographic index distribution curves before and after sink filling. This therefore indicated that the sink-filling had the least influence on the original topography;
b) it presented only two sinks which could be easily identified and corrected manually, thus ensuring hydrological consistency;
c) previous research by Quinn and Beven (1993) using the Plynlimon catchments had also recommended a resolution of 50m or less in order to more accurately predict drainage flow paths and internal catchment validation.

Furthermore, the two sinks found are actually located on the catchment boundary. In such cases the *sink.for* algorithm does not automatically correct the sinks because it considers them as valid drainage outflow points for the catchment[1]. Manual correction was therefore the only solution to ensure hydrological consistency in this DEM.

In terms of future research, the results obtained indicate that the issue of generating hydrologically consistent DEMs from digitised input data still represents an unresolved problem. In the absence of more robust algorithms and/or of sufficiently accurate raw topographic data, modellers must take care in verifying that the sink-filling procedure does not compromise hydrological consistency.

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[1] The same problem applies to the ARC-INFO GRID sink filling functions.

5.2 Model Performance and Validation

5.2.1 Preliminary Evaluation of Model Performance

With regard to the preliminary evaluation of model performance (see Section 4.2) using only a spatially lumped K_0, various observations can be made. Based on the efficiency values shown in Tab. 5.2 for the Hafren 1986 simulations, we can observe that a decrease in SRMAX produced a noticeable increase in model efficiency, essentially due to an increase in the total simulated flow volumes. The decrease in SRMAX from 0.225 m to 0.0225m was associated with an increase in baseflow of 0.5-1% over the simulation year, and a corresponding reduction in saturation excess flow. However, there was a marked decrease in the total estimated actual evaporation, which was largely accounted for by an increase in the saturated zone recharge. The improved efficiency suggests that the smaller values of root zone storage (SRMAX) are producing a better simulation of the storage-discharge mechanism in the soil saturated zone. These smaller values indicate that there is less storage available for evapotranspiration with the result that larger volumes are transferred to the saturated zone and, ultimately, increase the total outflow volumes.

With regard to the m parameter, the larger value of 0.021 m consistently produced the best results in Tab. 5.2. For each of the three SRMAX values considered (0.0225m, 0.0899m, 0.225 m) the baseflow to saturation excess plus saturation from above was roughly equal to 12, whereas for m equal to 0.0093m the same ratio was approximately equal to 6. This result therefore indicates that in the presence of rainfall regimes that can vary from year to year, each value of m results in a characteristic baseflow to saturation flow ratio which reflects the storage-discharge mechanism for the catchment in a given year.

CATCHMENT & YEAR *Const. K0 soil distribution*	HAFREN - 86	HAFREN - 86	HAFREN - 86	HAFREN - 86	HAFREN - 86	HAFREN - 86
TOPMODEL Parameters						
m (m)	0.021	0.0093	0.021	0.0093	0.021	0.0093
SRMAX (m)	0.0225	0.0225	0.0899	0.0899	0.225	0.225
SKO (m/h)	889.7419	889.7419	889.7419	889.7419	889.7419	889.7419
T0=m*KO (m^2/h)	18.68	8.27	18.68	8.27	18.68	8.27
Gamma	4.75	5.56	4.75	5.56	4.75	5.56
MODEL EFFICIENCY	**77.91%**	**70.77%**	**70.91%**	**64.01%**	**63.80%**	**58.73%**
FLOW COMP. TOTALS (and % of total sim. flow)						
SAT. ZONE RECHARGE (m)	1.100	1.021	0.955	0.882	0.849	0.782
BASEFLOW (m)	1.062 / 92.47	1.008 / 85.90	0.917 / 92.26	0.868 / 85.23	0.811 / 91.98	0.768 / 84.75
SAT. EXCESS FLOW (m)	0.083 / 7.19	0.143 / 12.23	0.074 / 7.40	0.129 / 12.69	0.067 / 7.63	0.118 / 13.05
SAT. FROM ABOVE (m)	0.004 / 0.34	0.022 / 1.88	0.003 / 0.35	0.021 / 2.08	0.003 / 0.39	0.020 / 2.19
WATER BALANCE						
TOTAL SIMULATED FLOWS (m)	1.149	1.173	0.994	1.018	0.882	0.907
TOTAL OBSERVED FLOWS (m)	1.339	1.339	1.339	1.339	1.339	1.339
TOTAL RAINFALL (m)	1.743	1.743	1.743	1.743	1.743	1.743
TOTAL POTENTIAL ET (m)	1.057	1.057	1.057	1.057	1.057	1.057
TOTAL PREDICTED ET (m)	0.556	0.556	0.711	0.711	0.823	0.823
FINAL BALANCE (m)	0.000	0.000	0.000	0.000	0.000	0.000

Table 5.2 – TOPMODEL Performance for Preliminary Runs: Constant K_0

The highest efficiency (77.91%) was obtained for values of m and SRMAX equal to 0.021m and 0.0225m respectively, for the Hafren 1986 data. From the point of view of consistency with field-based knowledge, such values are counterintuitive in the sense that:

a) one would expect a greater effective depth than 2.1 cm - which is the physical interpretation of m - through which the surface/subsurface runoff is transmitted;
b) the SRMAX value of 0.0225m, which includes both root zone and interception storage, seems very small for a forested catchment. Water balance studies carried out for the Plynlimon catchments estimate that for the forested Hafren, the transpiration loss alone is equal to 30-40% of rainfall, whereas for the grassland Gwy catchment the transpiration loss is only 15-20% of rainfall (Hudson et al., 1997)

Overall, these preliminary results supported the view that rather than dealing with fully physically-based parameters we were dealing with physically interpretable effective parameters. As such their optimal values could change from year to year, reflecting underlying changes in the catchment behaviour. What remained to be seen was what effect a spatially variable K_0 would have on parameter optimisation and resulting model performance.

5.2.2 Identification of Optimal Parameter Set

In order to establish a base case against which all the simulations with a spatially variable K_0 could be compared, the parameters (m, SRMAX, K_0) were optimised for the Hafren 1985 data. Results obtained from the iterative procedure indicated that (Tab. 5.3):

a) the three parameter values were not very physically realistic, with m and SRMAX very small and K_0avg very large with respect to expected field values;
b) TOPMODEL seemed relatively insensitive to large variations in K_0, as testified by the fact that the optimisation procedure only led to a marginal reduction in the initial range of K_0 values (Section 5.3).

Both of the above findings are confirmed by the results of other researchers (Robson et al., 1993; Quinn and Beven, 1993; Beven, 1997).

	Optimisation no.1	Optimisation no.2	Optimisation no.3
m (m)	0.01-0.1	0.01-0.014	0.01295-0.01362
SRMAX (m)	0.001-0.1	0.006-0.26	0.00603-0.0069
K_0 (m/hr)	885-895	885-895	886.436-893.292

Table 5.3 – Parameter ranges used in successive optimisations

From the split sample validation exercise carried out with the optimised parameters using the Hafren 1984 and 1986 data, and the Upper Hore 1985 data (see Tab. 5.4), some important observations can be made.

1) From only three years of data and two catchments it is not really possible to validate the optimised parameter set. The presence of continuing land use change (eg. forest felling in the Hafren) makes it difficult to define any one year as a base case parameter set.
2) The model efficiencies obtained for the Hafren 1985, 1986 and Upper Hore 1985 simulation periods are very similar ($\Delta \sim 1.5\%$), and the same is true for the baseflow component percentages. By contrast, the larger variation in the saturation excess flow components ($\Delta \sim 3.4\%$) may be caused by internal model fluctuations rather than actual changing catchment conditions. The presence of an intrinsic

variability in the flow component percentages from year to year indicates that it may not be possible to attribute changes in flow solely to the introduction of a spatially variable K_0. Also, such variability raises the question of how differences in component flows may affect the prediction of spatially distributed soil moisture deficits, which can only be verified by field measurements.

CATCHMENT & YEAR *Const. K0 Soil Distribution*	HAFREN 1985	UPPER HORE 1985	HAFREN 1986	HAFREN 1984
TOPMODEL Parameters				
m (m)	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616
KO (m/h)	890.978	890.978	890.978	890.978
T0=m*KO (m^2/h)	11.761	11.761	11.761	11.761
Gamma	5.304	4.993	5.304	5.304
MODEL EFFICIENCY	**85.40%**	**85.20%**	**84.96%**	**72.92%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW				
SAT. ZONE RECHARGE (m)	0.933	0.946	1.211	0.859
BASEFLOW (m)	.956 / 90.33	.969 / 89.20	1.189 / 88.82	.853 / 102.46
SAT. EXCESS FLOW (m)	.078 / 7.40	.065 / 5.96	.125 / 9.36	.074 / 8.86
SAT. FROM ABOVE (m)	.004 / .39	.004 / .40	.011 / .85	.006 / .66
WATER BALANCE				
TOTAL SIMULATED FLOWS (m)	1.039	1.038	1.326	0.933
TOTAL OBSERVED FLOWS (m)	1.058	1.086	1.339	0.833
TOTAL RAINFALL (m)	1.431	1.431	1.743	1.284
TOTAL POTENTIAL ET (m)	1.009	1.009	1.057	1.271
TOTAL PREDICTED ET (m)	0.415	0.415	0.395	0.349
FINAL BALANCE (m)	-0.001	-0.001	0.000	-0.005

Table 5.4 – Summary of Catchment Results with Constant K_0

3) The drop in efficiency for the Hafren 1984 simulation period is associated with a significant overestimate of the baseflow component, which is alone greater than the total observed flow. Based on the results for the other years, this would imply that model performance can only improve by decreasing baseflow
4) The efficiencies for Hafren 1985 and Upper Hore 1985 are very similar therefore confirming that, at least within identical simulation periods, the model performance is comparable over catchments of different spatial extent, but with similar physical characteristics. On the basis of these results, model performance does not appear to be scale dependent.

These initial observations therefore form the basis against which the results obtained for spatially variable K_0 distributions will now be examined.

5.2.3 Simulations with Published Saturated Conductivities

The simulations with the saturated conductivity values taken from literature were carried out:

a) to evaluate model performance, using the optimised (m, SRMAX) values which were considered to be constant for the catchment;

b) to evaluate if re-optimising the (m, SRMAX) values could provide improved model efficiencies with respect to a constant K_0.

As the results summarised in Tab. 5.5 show, the first conclusion that could be drawn was that the published values used for distributing K_0 (LITT. 1, LITT. 2) both led to totally unacceptable model predictions. Though the total simulated flows were very close to the total observed flows for Hafren 1985, the flow component breakdown showed a strong predominance of saturated flows compared to baseflow. The examination of the hydrographs (Section 4.4, Fig. 4.10) further revealed that while the timing and the magnitude of the flood peaks was not excessively in error, there were essentially no recession limbs in the predicted flood hydrographs.

CATCHMENT & YEAR *Soil Distribution*	HAFREN - 85 *Const. K0*	HAFREN - 85 *LITT. 1*	HAFREN - 85 *LITT. 2*	HAFREN - 85 *LITT. 1 Optim.*	HAFREN - 85 *LITT. 2 Optim.*
TOPMODEL Parameters					
m (m)	0.0132	0.0132	0.0132	0.88026	0.98458
SRMAX (m)	0.00616	0.00616	0.00616	0.12743	0.15666
K0 (m/h)	890.978	n.a.	n.a.	n.a.	n.a.
T0=m*KO (m^2/h)	11.761	0.009	0.005	0.588	0.400
Spatially Avg. K0	n.a	0.667823	0.406416	0.667823	0.406416
Gamma	5.212	12.565	13.234	8.364	8.924
MODEL EFFICIENCY	**85.40%**	**-387.60%**	**-417.17%**	**25.99%**	**7.51%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW					
SAT. ZONE RECHARGE (m)	0.933	0.095	0.067	0.431	0.324
BASEFLOW (m)	.956 / 90.33	.133 / 12.59	.109 / 10.31	1.075 / 101.56	1.077 / 101.76
SAT. EXCESS FLOW (m)	.078 / 7.40	.906 / 85.63	.932 / 88.04	.180 / 16.99	.265 / 25.04
SAT. FROM ABOVE (m)	.004 / .39	.014 / 1.34	.017 / 1.59	.000 / .02	.000 / .00
WATER BALANCE					
TOTAL SIMULATED FLOWS (m)	1.039	1.054	1.058	1.255	1.342
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058	1.058	1.058
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.820	0.842
FINAL BALANCE (m)	-0.001	-0.001	-0.001	-0.001	-0.001

Table 5.5 – Simulations with Published K_0 Distributions

The single most important factor influencing these results was the difference in the soil-topographic index distributions (see Fig. 5.1) which led to area weighted averages of K_0 that were roughly three orders of magnitude smaller with respect to the calibrated K_0avg. This lead to much higher values of gamma (γ), which is a fundamental parameter in the calculation of the local soil moisture deficits:

$$S_i = SBAR - m[\gamma - \ln(a/T_0 \tan\beta)_i] \quad \text{(Eqn. 5.1)}$$

As gamma increases, the above relationship shows that the local soil moisture deficit (S_i) decreases, therefore increasing the likelihood of saturated excess flow with respect to baseflow and this is exactly what Tab. 5.5 shows.

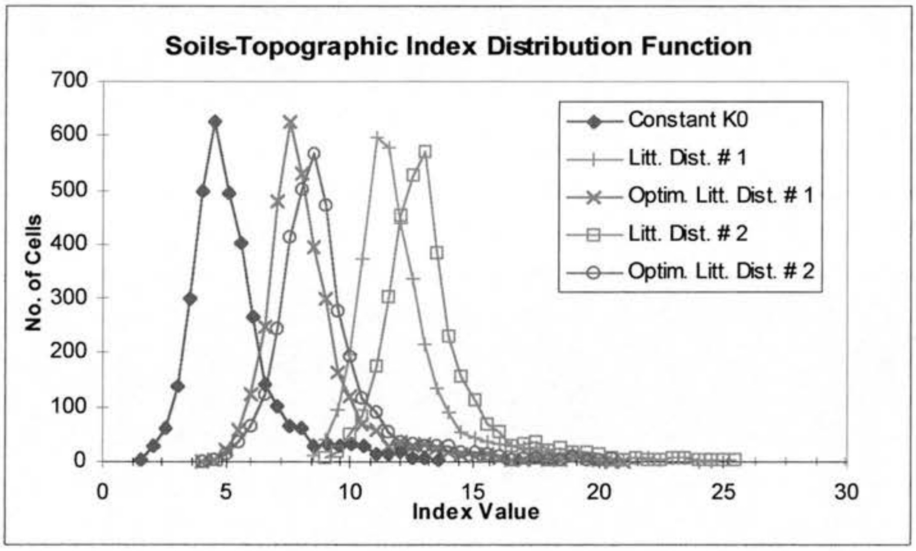


Figure 5.1 – Soil-Topographic Index Distribution: LITT.1 & LITT.2

Given the findings with the published K_0 values, the question arose of whether there might exist a point in the (m, SRMAX) parameter space that would provide better model predictions. The model parameters were therefore re-optimised for each of the published K_0 distributions. While the reoptimised model efficiencies were significantly better, and the flow component breakdown was much closer to that obtained for constant K_0, the model overestimated the total observed flows by 20-30%. Also, the hydrographs showed a marked increase in the baseflow component which was unrealistic. This increase can be explained by examining the plots of the soil-topographic index distributions shown in Fig. 5.1. As the topographic index distribution [ln(a/tanß)] is fixed for a given catchment and resolution, the soil-topographic index value and its' catchment average value, gamma, was controlled by the values of K_0 and m through the following equation.

$$\ln(a/T_0 \tan\beta) = \ln(a/\tan\beta) - \ln(T_0) = \ln(a/\tan\beta) - \ln(m\, K_0) \qquad \text{(Eqn. 5.2)}$$

The higher values of the reoptimised (m) parameter did help to reduce the values of the soil-topographic index and, therefore, of gamma. This led to a decrease in the saturation excess flow component and an increase in the baseflow component. Also, the significant increase in SRMAX led to simulated ET values which were much closer to potential ET. But overall, the combined effect of m and SRMAX was still not enough to compensate for the very small spatially averaged K_0 in both LITT.1 and LITT.2., and in both cases this led to overestimations of the total simulated flows.

Finally, it is interesting to note how the re-optimised (m, SRMAX) values are actually intuitively more physically realistic, at least with respect to field-based knowledge of the catchments. This raises the question of whether soil K_0 distributions derived from a comprehensive field sampling exercise for the chosen catchment might not have led to better model performance.

Based on the results obtained using the published K_0 values, we can only conclude that there has been no improvement in model performance with respect to the results with a constant K_0. Furthermore, the results again underline the role of K_0 as an effective parameter which does not necessarily reflect field conditions.

5.2.4 Simulations with Scaled Saturated Conductivities

If K_0 was to be considered as an effective parameter, then it was logical to attempt to normalise all of the chosen K_0 distributions, so that their results could be compared. The scaling was carried out so that the area weighted average would coincide with the calibrated K_0avg. As was to be expected, once the scaling of K_0 was carried out the model performance - at least in terms of outflow prediction - became very similar for the various K_0 distributions (Tab. 5.6). The simulations also confirmed that the highest efficiencies were associated with the K_0 distributions which determined soil-topographic index distributions most similar to the case of a constant K_0.

For the Hafren 1984-86 simulations the highest efficiencies were always obtained for a constant K_0, with the HOST-SPR distribution giving the next best results. In terms both of total simulated flows and predicted hydrographs, the two cases gave virtually identical results.

CATCHMENT & YEAR	HAFREN - 85	HAFREN - 85	HAFREN - 85	HAFREN - 85	HAFREN - 85
Soil Distribution	*Const. K0*	*LITT. 1*	*LITT. 2*	*Wetness Class*	*HOST-SPR*
TOPMODEL Parameters					
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	890.978	890.978	890.978	890.978
T0=m*KO (m^2/h)	11.7609	11.7618	11.7618	11.7610	11.7610
Spatially Avg. K0 (m)	n.a	891.026	891.030	890.964	890.981
Gamma	5.212	5.370	5.543	5.328	5.328
EFFICIENCY '85	**85.40%**	**85.20%**	84.87%	85.19%	**85.20%**
EFFICIENCY '86	**84.96%**	84.60%	83.64%	84.73%	**84.77%**
EFFICIENCY '84	**72.92%**	72.35%	71.16%	72.53%	**72.58%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW					
SAT. ZONE RECHARGE (m)	0.933	0.924	0.914	0.924	0.924
BASEFLOW (m)	.956 / 90.33	.947 / 89.51	.938 / 88.60	.947 / 89.51	.947 / 89.52
SAT. EXCESS FLOW (m)	.078 / 7.40	.087 / 8.18	.096 / 9.08	.087 / 8.21	.087 / 8.19
SAT. FROM ABOVE (m)	.004 / .39	.005 / .44	.005 / .45	.004 / .42	.004 / .42
WATER BALANCE					
TOTAL SIMULATED FLOWS (m)	1.039	1.039	1.039	1.039	1.039
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058	1.058	1.058
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.415	0.415
FINAL BALANCE (m)	-0.001	-0.001	-0.001	-0.001	-0.001

Table 5.6 – Simulations with Scaled K_0 Distributions: Hafren

Purely for model verification purposes, the parameters (m, SRMAX, K_0avg) were reoptimised. Given that the scaling of the K_0 distributions had already led to a normalisation of all the distributions, large variations in the new parameters and in model performance with respect to the constant K_0 case were not to be found, as was expected.

Going on to examine the Upper Hore 1985 simulations (Tab. 5.7), the results essentially confirmed those already found for the Hafren. The main exception was in the fact that the highest model efficiencies were obtained with the LITT. 2 K_0 distribution, which predicted the highest percentage of saturated flow.

This can be explained in light of the fact that the LITT. 2 distribution uses depth-averaged K_0 values, which lead to much smaller K_0 values for the Hafren soils and slightly larger K_0 values for the Crowdy and Skiddaw soils (Section 4.5, Tab. 4.8). Though there is a higher prevalence of Crowdy soils in the Upper Hore subcatchment (56%) compared to the Hafren catchment (45%), the greater reduction in the Hafren soil K_0 values led to an increase in the catchment average value (gamma) of the soil-topographic index. Consequently, this resulted in a higher percentage of saturated runoff with respect to that predicted by the other distributions. But, as with the Hafren simulations, in terms of total simulated flows and predicted hydrographs the constant K_0, HOST-SPR and LITT. 2 distributions are essentially identical.

CATCHMENT & YEAR *Soil Distribution*	UPPER HORE - 85 *Const. K0*	UPPER HORE - 85 *LITT. 1*	UPPER HORE - 85 *LITT. 2*	UPPER HORE - 85 *Wetness Class*	UPPER HORE - 85 *HOST-SPR*
TOPMODEL Parameters					
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	890.978	890.978	890.978	890.978
T0=m*KO (m^2/h)	11.761	11.761	11.763	11.761	11.761
Spatially Avg. K0 (m)	n.a.	890.977	891.132	890.987	890.976
Gamma	4.993	5.003	5.152	5.008	5.008
EFFICIENCY '85	**85.20%**	85.20%	**85.40%**	85.17%	**85.19%**
EFFICIENCY HAFREN '85	**85.40%**	85.20%	**84.87%**	85.19%	**85.20%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW					
SAT. ZONE RECHARGE (m)	0.946	0.945	0.933	0.944	0.945
BASEFLOW (m)	.969 / 89.20	.967 / 89.08	.956 / 88.01	.967 / 89.03	.967 / 89.05
SAT. EXCESS FLOW (m)	.065 / 5.96	.066 / 6.11	.077 / 7.11	.067 / 6.17	.067 / 6.15
SAT. FROM ABOVE (m)	.004 / .40	.004 / .37	.005 / .44	.004 / .36	.004 / .37
WATER BALANCE					
TOTAL SIMULATED FLOWS (m)	1.038	1.038	1.038	1.038	1.038
TOTAL OBSERVED FLOWS (m)	1.086	1.086	1.086	1.086	1.086
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.415	0.415
FINAL BALANCE (m)	-0.001	-0.001	-0.001	-0.001	-0.001

Table 5.7 – Simulations with Scaled K_0 Distributions: Upper Hore

The simulations with scaled K_0 distributions have shown that in terms of predicted outflows, the inclusion of a spatially variable K_0 does not significantly affect model performance either at the catchment or the subcatchment scale. The fact that the Upper Hore efficiencies are so similar with respect to the Hafren catchment simulations is not surprising given that the index distribution curves for the two catchments are quite similar, as shown in Fig. 5.2. Though the differences in the lower index values lead to noticeable variations in the gamma values for the two catchments, the similarity in the higher index values is sufficient to determine the similarity in model efficiencies and total predicted simulated flows.

Furthermore, it is important to underline that the normalisation of the variable K_0 distributions with respect to the calibrated K_0avg has further contributed to minimising the variation in the predicted flow components, within each of the two catchments. Yet the decision to normalise the variable K_0 distributions was forced by the effective nature of the K_0 parameter. The simulations with the LITT.1 and LITT.2 distributions proved that published K_0 values did not lead to realistic model results. As a result, the need to use surrogate indeces – which are themselves effective parameters – required normalisation to be carried out in order to make the simulation results comparable.

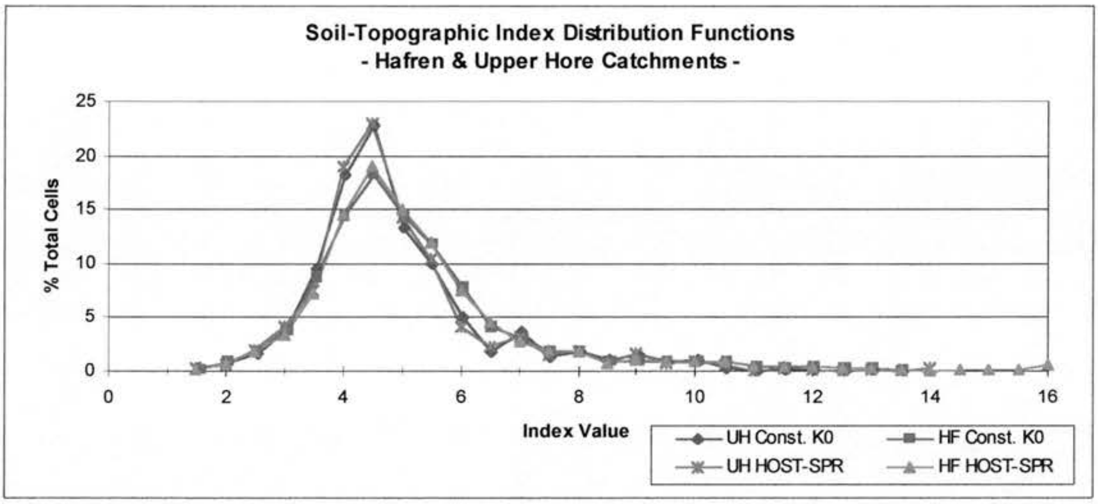


Figure 5.2 – Soil-Topographic Index Distribution: Constant and HOST SPR K_0

This result seems to indicate that for the range and type of catchment sizes chosen, model performance is not scale dependent. Furthermore, because the soil-topographic index curves are so similar, there will not be any noticeable difference in the spatial distribution of soil moisture deficit, especially at the higher index values.

5.2.5 Simulations considering a Channel Initiation Threshold

The main objective of the CIT method, and other similar methods (Saulnier et al., 1997a), is to distinguish the hillslope cells from the drainage network cells. In this way the wetness index distribution function - in this case defined by the soil-topographic index - will not be biased by the presence of cells containing channel elements. For such cells, the actual drained area will coincide with the hillslope area draining directly to the channel, rather than with all of the upstream area drained by the cell. The latter case is the default in the standard TOPMODEL code and has been referred to as the CIT_{∞} case, indicating that the CIT value is greater than the catchment area and therefore no cell can ever be a drainage network cell.

Once an appropriate CIT value had been identified for the Hafren catchment[2], equal to 25,000 m^2, two different methods were considered for calculating the modified topographic index. The first method is described by Quinn et al. (1995a) and simply uses a modified equation for the topographic index, for those cells for which a > CIT. The equation used is based on the geometrical configuration shown in Fig. 4.14 where A is the upslope area and L is the channel length equal to the grid size.

A second method for calculating the topographic index was used, which simply eliminated any flagged cells having CIT > 25000m^2. Other methods could have been used to more accurately calculate the topographic index (eg. Saulnier et al., 1997a) but these two were chosen because it was felt that they represented the two solutions likely to result in the greatest difference to the calculated soil-topographic distribution functions.

From an examination of the modified soil-topographic distribution curves (see Figs. 5.3, 5.4) and of the simulation results summarised in Tab. 5.8, various observations can be made. The first observation regards the similarity in distribution curves and in the simulation results obtained with the two modified topographic index calculation methods (M1 and M2). Eliminating the river cells (M2) has reduced the number of valid catchment cells from 3463 to 2973 for the Hafren, and from 652 to 547 for the Upper Hore, which represents a reduction of 14% and 16% respectively. Yet the variations in model efficiencies are at most 2%. It therefore would appear that the

[2] Quinn et al. 1997 calculated CIT=22,500sq.m for the Gwy catchment

different treatment of river cells has not significantly altered the model's performance in terms of total predicted outflow.

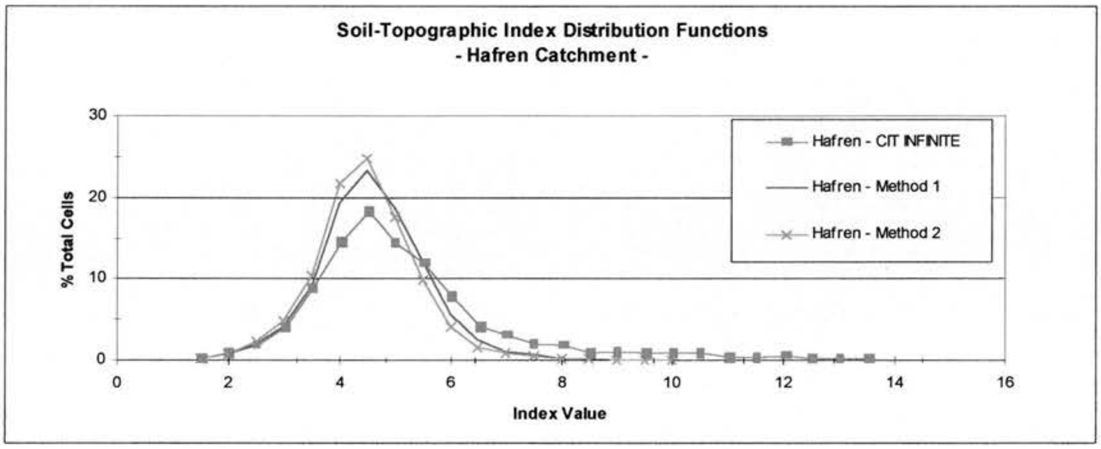


Figure 5.3 – Hafren Modified Soil-Topographic Index Distributions

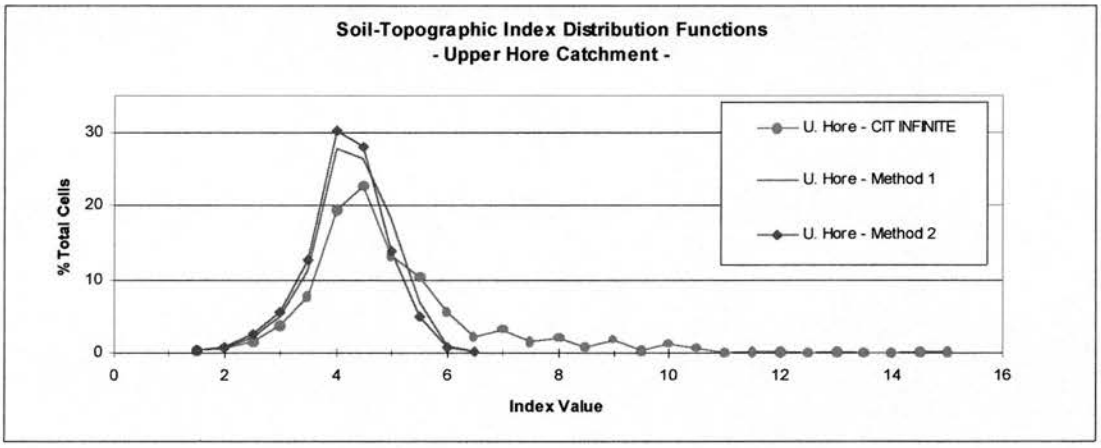


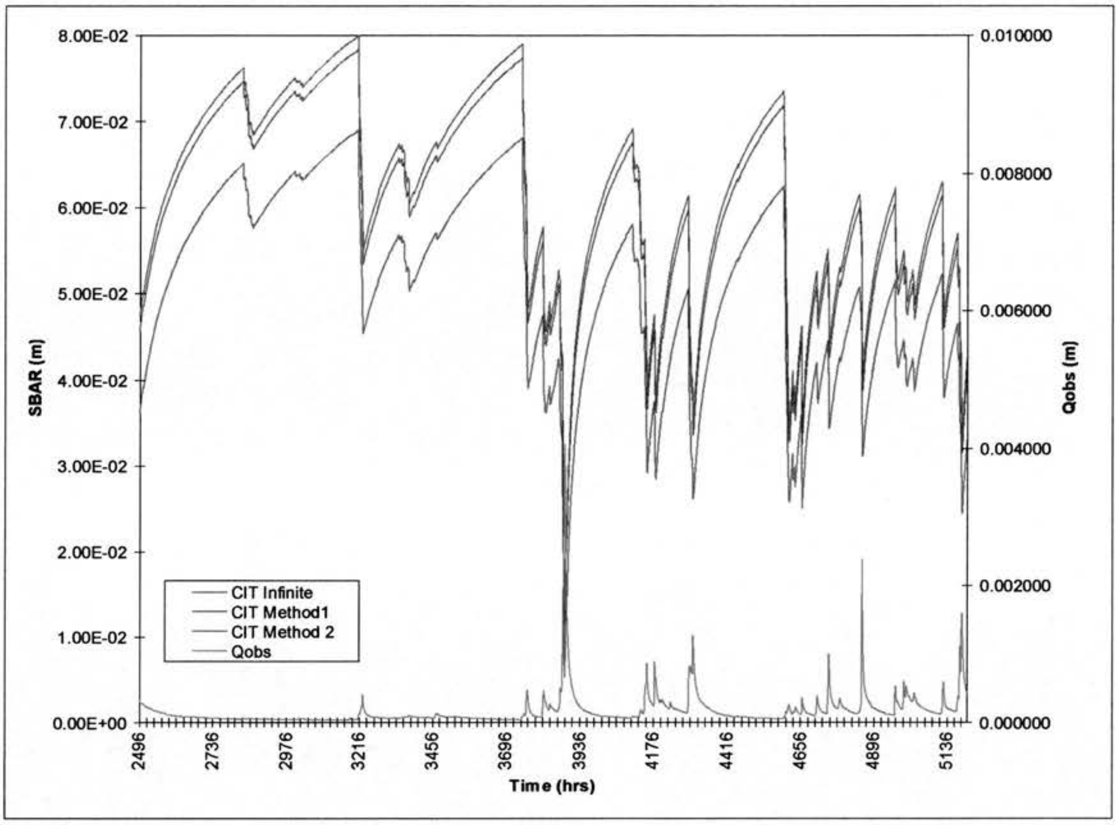
Figure 5.4 – Upper Hore Modified Soil-Topographic Index Distributions

CATCHMENT & YEAR (K0 HOST SPR) CIT = 25000 sq.m.	HAFREN - 85 CIT INFINITE	HAFREN - 85 Method 1	HAFREN - 85 Method 2	UPPER HORE - 85 CIT INFINITE	UPPER HORE - 85 Method 1	UPPER HORE - 85 Method 2
TOPMODEL Parameters						
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	890.978	890.978	890.978	890.978	890.978
T0=m*K0 (m^2/h)	11.7610	11.7610	11.7197	11.7609	11.7609	11.7535
Spatially Avg. K0 (m)	890.9811	890.9811	887.8453	890.9764	890.9764	890.4153
Gamma	5.328	4.604	4.483	5.008	4.279	4.184
EFFICIENCY	**85.20%**	**83.18%**	**83.00%**	**85.19%**	**81.19%**	**81.07%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW						
SAT ZONE RECHARGE (m)	0.924	1.004	1.006	0.945	1.014	1.015
BASEFLOW (m)	.947 / 89.52	1.027 / 97.01	1.029 / 97.18	.967 / 89.05	1.036 / 95.44	1.037 / 95.47
SAT. EXCESS FLOW (m)	.087 / 8.19	.009 / .85	.008 / .74	.067 / 6.15	.001 / .07	.001 / .05
SAT. FROM ABOVE (m)	.004 / .42	.003 / .25	.002 / .18	.004 / .37	.000 / .04	.000 / .03
WATER BALANCE						
TOTAL SIMULATED FLOWS (m)	1.039	1.038	1.038	1.038	1.038	1.038
TOTAL OBSERVED FLOWS (m)	1.058	1.058	1.058	1.086	1.086	1.086
TOTAL RAINFALL (m)	1.431	1.431	1.431	1.431	1.431	1.431
TOTAL POTENTIAL ET (m)	1.009	1.009	1.009	1.009	1.009	1.009
TOTAL PREDICTED ET (m)	0.415	0.415	0.415	0.415	0.415	0.415
FINAL BUDGET (m)	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001

Table 5.8 – Summary of Simulations using CIT Method

If we consider the values of gamma with respect to the CIT_{∞} case, the Method 1 and Method 2 simulations present a noticeable reduction in gamma (2-4%). This reduction leads to a lower likelihood of saturation for the catchment cells, and consequently to an increase in the Saturated Zone Recharge and Baseflow flow components. This effect however is not improving the model's representation of catchment processes, because the reduction in Saturation Excess Flow means that many of the predicted flood peaks are still underestimating the observed flow (see Figs. 4.18, 4.19).

There does though appear to have been an improvement in terms of the spiky nature of the predicted flow, compared to the flows obtained for CIT_{∞}. This can be explained by the lower values of the catchment average soil-topographic index (gamma) obtained with Method 1 and Method 2, which will lead to higher soil moisture deficits (see Eqn. 5.1) and a more limited extent of saturated areas which will result in less flashy runoff generation. This is confirmed by the consistently greater values of catchment average SMD (SBAR) obtained using the two CIT methods (Fig. 5.5).



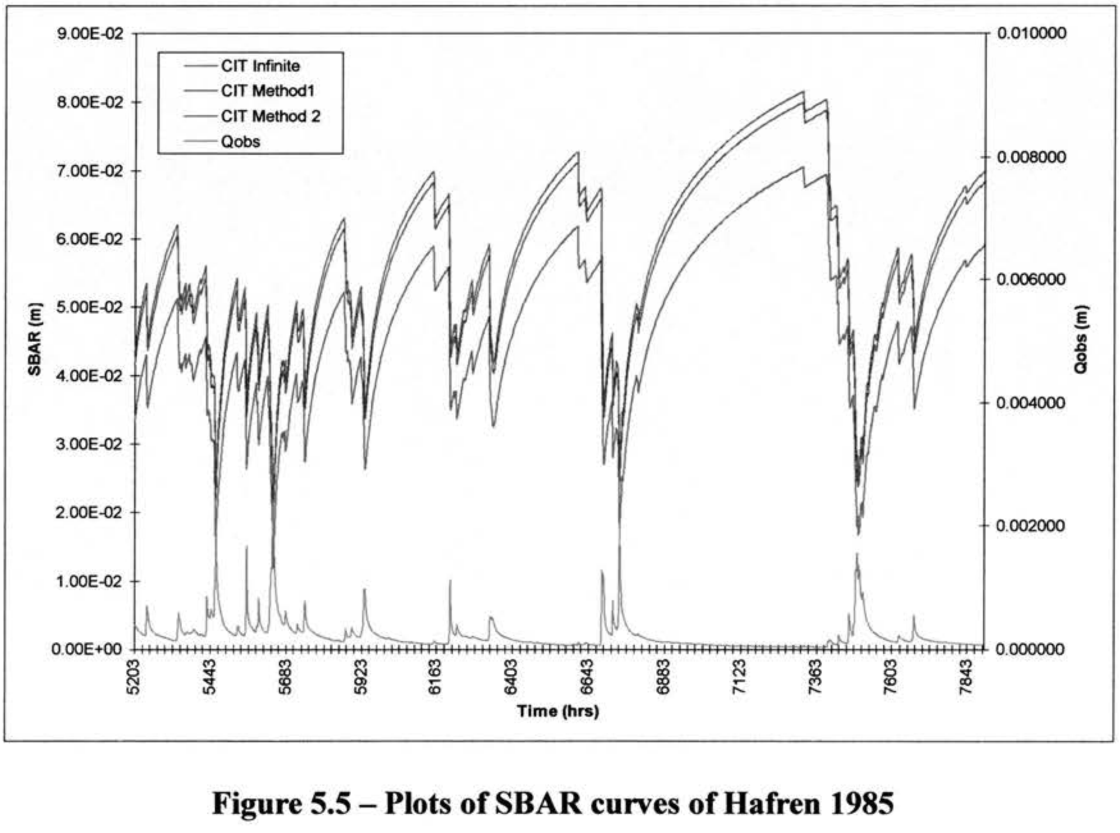


Figure 5.5 – Plots of SBAR curves of Hafren 1985

We can therefore conclude that adopting the CIT approach did not lead to improvements in TOPMODEL's predictions of catchment outflow. As shown by Tab. 5.8 the application of a CIT threshold did lead to a redistribution amongst the various flow components, but the overall total simulated flow remained unaltered. It may well be that the CIT method was not appropriate for these catchments because:

a) the relatively small number of cells containing channel elements were not sufficient to radically alter model performance;
b) the difficulty in simulating the catchments' response is associated with an underestimation in yearly saturated flows, so that any method which increases the baseflow component will not actually improve the results.

Using the CIT approach may modify the spatio-temporal distribution of the soil moisture deficit values for single events, but the higher values of mean SMD (SBAR) would generally lead to less saturated conditions throughout the catchment. Given that the chosen catchments are strongly controlled by the behaviour of the upland peats and how they affect saturation patterns, the CIT methods were not used for the single event SMD simulations.

5.2.6 Simulations of Single Flood Events

After having carried out the simulations described in the preceding sections, it was clear that the adoption of a spatially variable K_0 was not having any significant effect on the model performance with respect to catchment outflow. The question that remained to be answered was whether an examination of specific flood events and, more importantly, the associated soil moisture deficit maps would highlight any significant differences between the constant K_0 and the spatially variable K_0 simulation results. This section will examine the question in relation to the predicted hydrographs, while the following section will consider the implications for soil moisture deficit.

The events were all chosen from the late spring and summer months of the 1985 simulation period, on the assumption that the soil moisture deficit would show a wide range of variation between the minimum and maximum flows. From an examination of the event hydrographs, the catchment average SMD (SBAR) curve (Fig. 5.6) and the summary tables (Tab. 5.9, 5.10) some general conclusions can be drawn.

HAFREN 1985	**EVENT 1 (3854-4099)**		**EVENT 2 (4307-4776)**		**EVENT 3 (4803-4962)**		**EVENT 4 (5476-5865)**	
Soil Distribution	***Const. K0***	***HOST SPR***	***Const. K0***	***HOST SPR***	***Const. K0***	***HOST SPR***	***Const. K0***	***HOST SPR***
TOPMODEL Parameters								
m (m)	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	890.978	n.a.	890.978	n.a.	890.978	n.a.	890.978	n.a.
T0=m*KO (m^2/h)	11.761	11.761	11.761	11.761	11.761	11.761	11.761	11.761
Spatially Avg. K0	n.a.	890.981	n.a.	890.981	n.a.	890.981	n.a.	890.981
Gamma	5.212	5.328	5.212	5.328	5.212	5.328	5.212	5.328
EFFICIENCY '85	**97.41%**	**97.50%**	**-52.65%**	**-53.39%**	**54.61%**	**55.91%**	**91.38%**	**90.86%**
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW								
SAT. ZONE RECHARGE (m)	0.066	0.066	0.082	0.081	0.022	0.022	0.113	0.112
BASEFLOW (m)	.080 / 93.75	.080 / 93.20	.102 / 135.16	.101 / 134.25	.031 / 77.56	.031 / 77.13	.138 / 88.93	.137 / 88.31
SAT. EXCESS FLOW (m)	.011 / 13.40	.012 / 13.65	.006 / 8.17	.007 / 9.24	.002 / 3.88	.002 / 4.24	.012 / 7.48	.013 / 8.13
SAT. FROM ABOVE (m)	.001 / 1.24	.001 / 1.54	.000 / .53	.000 / .49	.000 / .23	.000 / .39	.001 / .39	.001 / .39
WATER BALANCE								
TOTAL SIMULATED FLOWS (m)	0.093	0.093	0.109	0.109	0.032	0.032	0.150	0.150
TOTAL OBSERVED FLOWS (m)	0.086	0.086	0.075	0.075	0.040	0.040	0.155	0.155
TOTAL RAINFALL (m)	0.089	0.089	0.128	0.128	0.031	0.031	0.173	0.173
TOTAL POTENTIAL ET (m)	0.073	0.073	0.158	0.158	0.043	0.043	0.062	0.062
TOTAL PREDICTED ET (m)	0.016	0.016	0.048	0.048	0.014	0.014	0.048	0.048
FINAL BUDGET	-0.013	-0.013	-0.018	-0.018	-0.011	-0.011	0.000	0.000

Table 5.9 – Summary of Hafren Event Simulations

UPPER HORE 1985	**EVENT 1 (3854-4099)**	**EVENT 2 (4307-4776)**	**EVENT 3 (4803-4962)**	**EVENT 4 (5476-5865)**
Soil Distribution	***HOST SPR***	***HOST SPR***	***HOST SPR***	***HOST SPR***
TOPMODEL Parameters				
m (m)	0.0132	0.0132	0.0132	0.0132
SRMAX (m)	0.00616	0.00616	0.00616	0.00616
K0 (m/h)	n.a.	n.a.	n.a.	n.a.
T0=m*KO (m^2/h)	11.7609	11.7609	11.7609	11.7609
Spatially Avg. K0 (m)	890.9764	890.9764	890.9764	890.9764
Gamma	4.985	4.985	4.985	4.985
EFFICIENCY '85	**95.98%**	**-6.89%**	**45.72%**	**91.81%**
EFFICIENCY HAFREN '85	97.50%	-53.39%	55.91%	90.86%
FLOW COMP. TOTALS / % OF TOTAL OBS. FLOW				
SAT. ZONE RECHARGE (m)	0.068	0.083	0.022	0.115
BASEFLOW (m)	.083 / 94.27	.103 / 130.18	.031 / 74.38	.138 / 89.51
SAT. EXCESS FLOW (m)	.009 / 10.72	.005 / 6.61	.001 / 3.18	.010 / 6.54
SAT. FROM ABOVE (m)	.001 / 1.20	.000 / .46	.000 / .20	.000 / .30
WATER BALANCE				
TOTAL SIMULATED FLOWS (m)	0.094	0.109	0.033	0.149
TOTAL OBSERVED FLOWS (m)	0.088	0.079	0.042	0.155
TOTAL RAINFALL (m)	0.089	0.128	0.031	0.173
TOTAL POTENTIAL ET (m)	0.073	0.158	0.043	0.062
TOTAL PREDICTED ET (m)	0.016	0.048	0.014	0.048
FINAL BUDGET	-0.013	-0.018	-0.011	0.000

Table 5.10 – Summary of Upper Hore Event Simulations

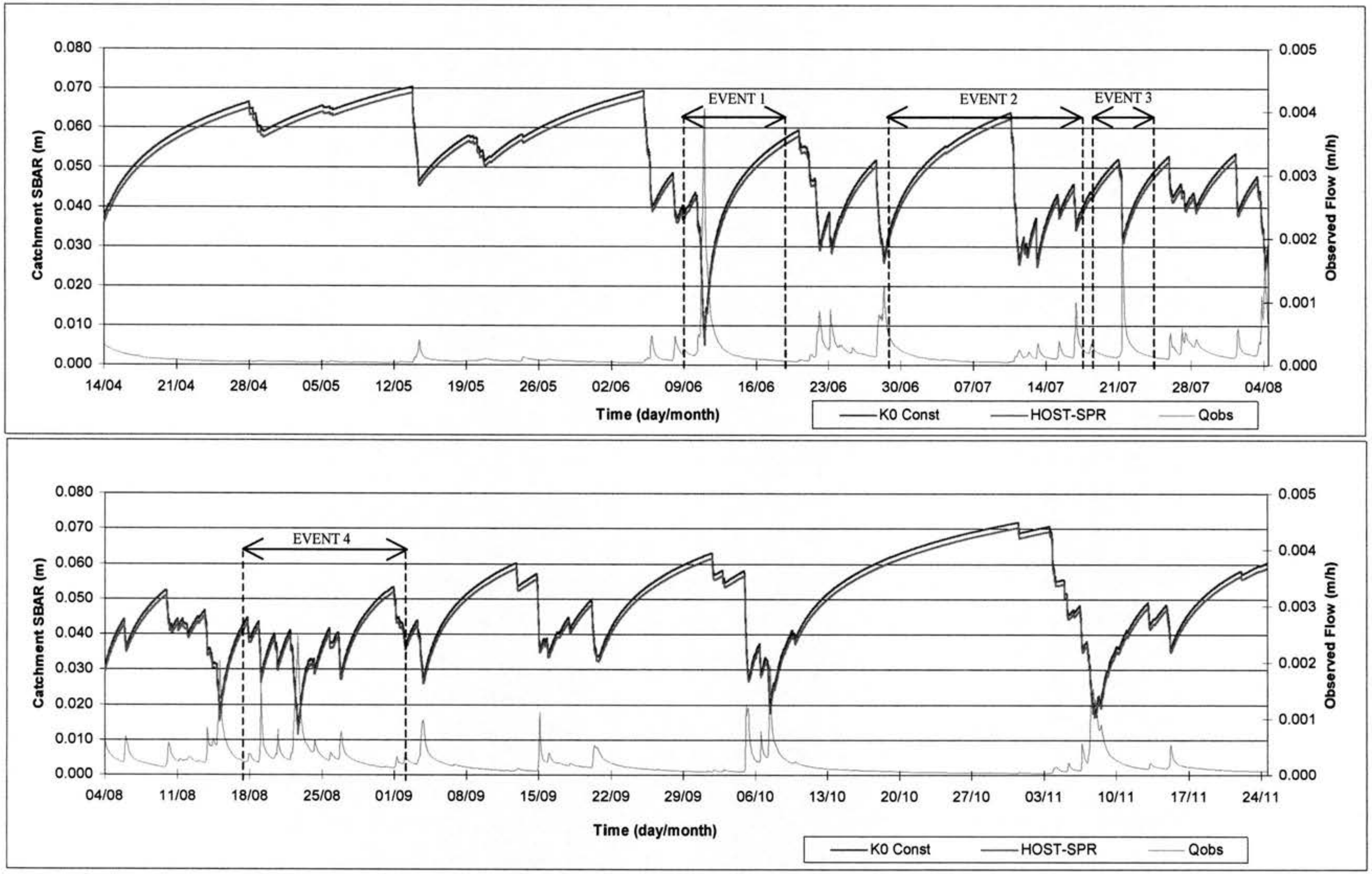


Figure 5.6 - Catchment SBAR Curves - Hafren 1985

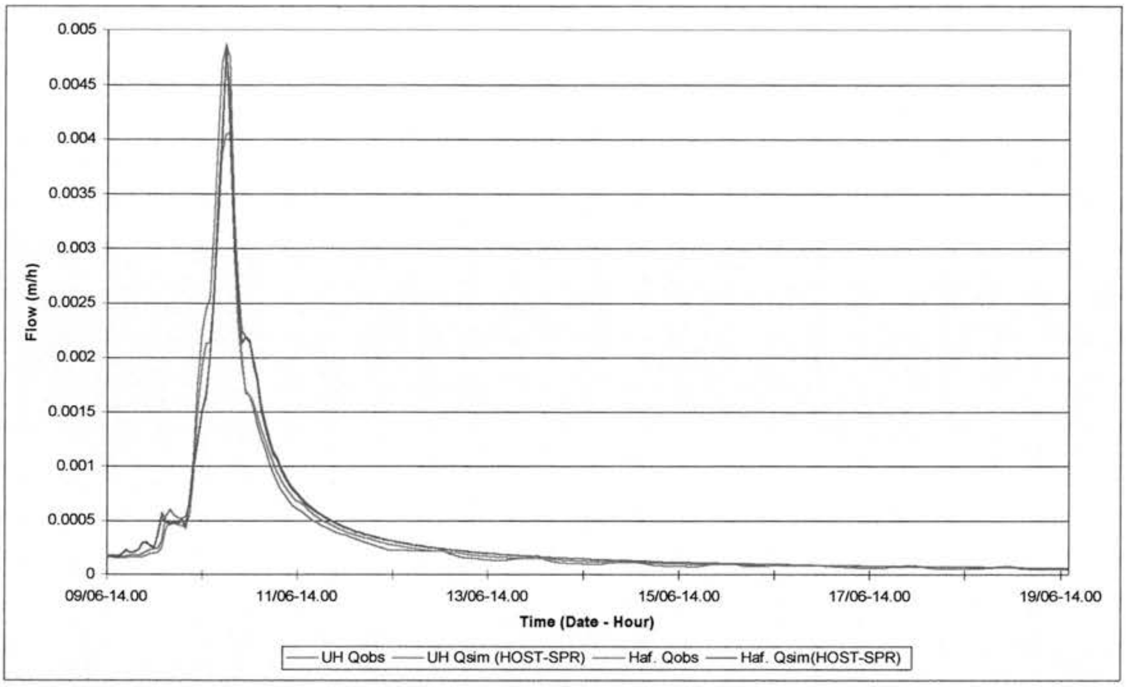


Figure 5.7 – Hydrographs for Event 1

The variable K_0 (HOST-SPR distribution) simulations for Event 1 presented the highest efficiencies for both the Hafren (97%) and the Upper Hore (96%), which were accompanied by higher baseflow component percentages – 93% and 94% respectively – than those found for the entire 1985 simulation period (~90%).

The relatively high saturated flow component percentages in the Hafren and Upper Hore- 15% and 12% respectively - were accompanied by an overestimation of total simulated flows for both catchments. The fact that the total simulated flows are greater than the observed flows can be attributed to increases in both the baseflow and the saturation flow components. Given that all of the events being simulated are flood events, which are generally associated with significant increases in the saturated flow components, the high baseflow values found for both the Hafren and the Upper Hore appear excessive in terms of contribution to total simulated flows.

There is also a negative Final Budget[3] value (-0.013 m) for both catchments, indicating a predicted net loss of water from the catchments. This last result should not be considered as an absolute error, but rather as an indication of the behaviour of the model with respect to the storage and release of water volumes.

In this respect, it is important to observe that this event was preceded by approximately 5 days of rainfall, during which the catchment average soil moisture deficit underwent a noticeable reduction (Fig. 5.6) and the volume of water stored in the saturated zone would have increased accordingly. Consequently, when Event 1 occurred the catchment released water which had been previously stored in the soils and this is reflected by the negative Final Balance. From an examination of the SBAR curve in Fig. 5.6, we can also observe that the catchment average SBAR value at the beginning of the event and during the rising limb is never greater than 0.045 m.

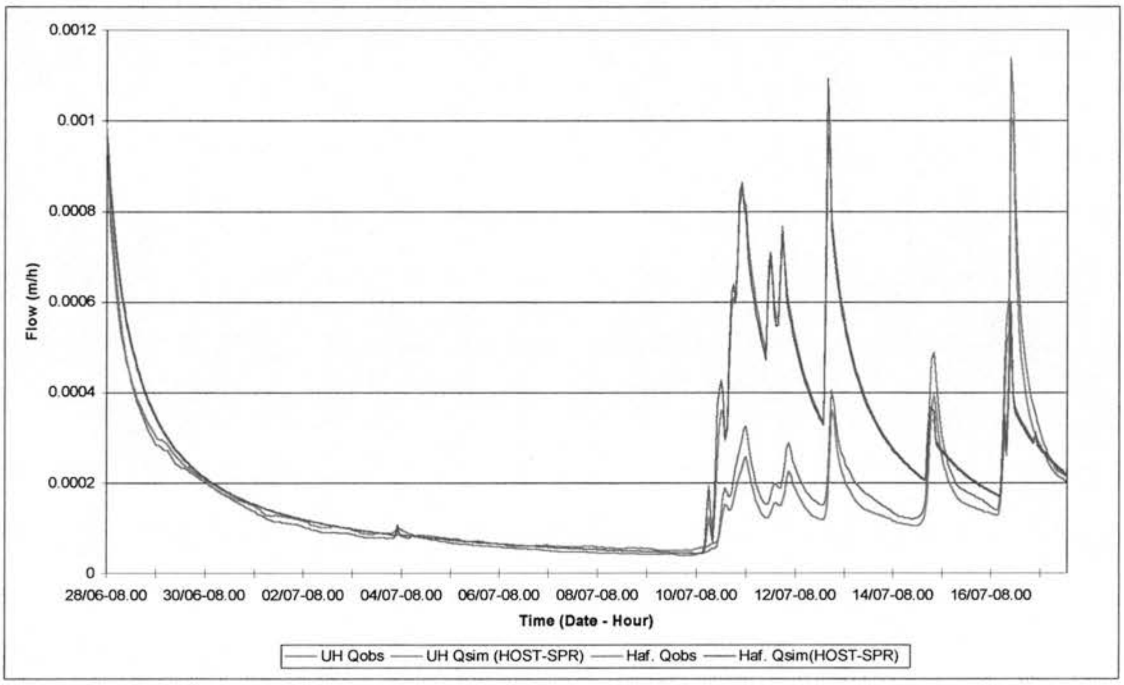


Figure 5.8 – Hydrographs for Event 2

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[3] The final budget is calculated by summing all the precipitation, runoff, evapotranspiration and soil storage components (see Section 3.3.6).

The Event 2 simulations for variable K_0 (HOST-SPR distribution) instead show the worst efficiencies for both the Hafren (-53.39%) and the Upper Hore (-6.89%). Nonetheless, this event is probably the one that is most helpful in understanding the manner in which TOPMODEL simulates catchment runoff processes. We should first of all recall (Section 3.9.1) that while ideally we should strive for efficiencies of 100%, it is possible to obtain negative values. Due to the structure of the efficiency equation, negative values occur when the variance of the residual error (Qsim-Qobs) of the simulated flows is greater than the variance of the observed flows. This in turn indicates a very low level of accuracy, even though the total simulated flows may still be comparable to the observed flows (see Table 5.5).

The negative efficiencies for Event 2 are accompanied by unrealistically high baseflow component percentages - 134% and 130% respectively - which are greater than the total observed flows. Again there is a negative Final budget value for both catchments, which is indicating that the model is releasing more water than is being input during the event. The plot of the flow hydrographs (Fig. 5.8) confirms that the model is not correctly simulating the events because:

1. the calculated flows from the beginning of the flood event to the beginning of the flood event on 15th July are approximately three times the observed values;
2. only for the two final flood peaks is the observed flow equal to or greater than the simulated flow, with the Upper Hore simulations showing the greater difference.

Given the reasonably good match to the recession flows preceding the flood event, we can only conclude that the catchment is showing a delayed response with respect to the flows predicted by the model, and temporarily storing internally a certain volume of water. This could be due to:

a) the catchment blanket peats accumulating water without releasing it immediately;
b) the saturated runoff generating areas not exhibiting sufficient spatial connectivity to allow rapid transfer of surface water to the catchment outflow.

The first reason would be consistent with the generally held view that peat is very efficient at storing water until it reaches a critical water content threshold, at which point it starts releasing water. In this case, both the release of water by the peats and the extensive spatial connectivity of the saturated areas occurs from the flood event of 15^{th} July onwards, when there is a significant increase in the observed flows. From an examination of the SBAR curve in Fig. 5.6 it would also appear that such an increase is associated with a catchment average soil moisture deficit value value of approximately 0.045 m at the beginning of the flood peak.

Unfortunately, both of the runoff generating mechanisms described above are not represented within the logic of TOPMODEL, which assumes a constant rate of drainage of the saturated zones through the baseflow component, and permanently connected saturated areas. We shall return to these two points for the other simulated events and when we consider the SMD maps in the following section.

The higher observed flows for the Upper Hore compared to the Hafren, for all of the flood peaks, further confirms that the model is not correctly simulating actual catchment behaviour. The observed flows indicate that the subcatchment is releasing greater flows per unit area than the whole of the Hafren. Intuitively, we would expect the Upper Hore soils to be generally wetter – given the more extensive presence of blanket peats (56% of Upper Hore area vs. 45% of Hafren area) - and therefore of responding more quickly to precipitation events. Yet TOPMODEL simulates flows per unit area from the Hafren and the Upper Hore as virtually identical.

The Event 3 simulations for variable K_0 (HOST-SPR distribution) showed quite low efficiencies for both the Hafren (56%) and the Upper Hore (46%). These results were accompanied by the lowest baseflow component percentages of all four events, equal to 77% and 74% respectively. The event totals show an underestimation of total predicted flows, equal to approximately -20%. Yet the presence of a negative Final budget again indicates that the model is releasing more water than is being stored. The plot of the flow hydrographs (Fig. 5.9) confirms that the model is not correctly simulating the event because it is clear that the predicted flows are not matching the full increase in observed flows, while nonetheless correctly predicting the recession limbs preceding and following the flood peak.

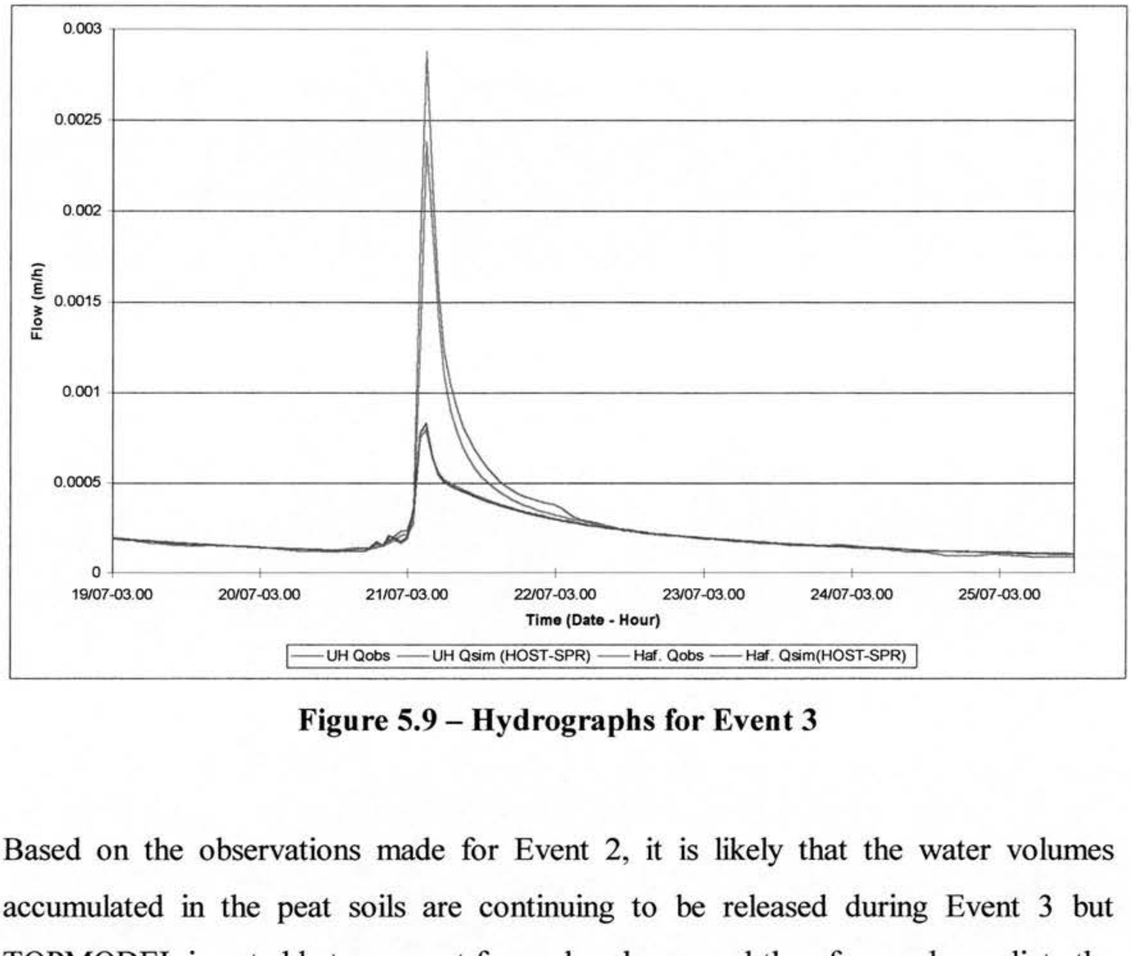

Figure 5.9 – Hydrographs for Event 3

Based on the observations made for Event 2, it is likely that the water volumes accumulated in the peat soils are continuing to be released during Event 3 but TOPMODEL is not able to account for such volumes and therefore underpredicts the flood peak. Also, from an examination of the catchment SBAR curve in Fig. 5.6 we can see that at the beginning of the flood peak the SBAR value is approximately 0.05 m, which is a value similar to that observed for Events 1 and 2.

The Event 4 simulations for variable K_0 (HOST-SPR distribution) showed quite high efficiencies for both the Hafren (90.86%) and the Upper Hore (91.81%). These results were accompanied by baseflow component percentages very close to the full year simulations - 88% and 90% respectively. The event totals show a slight underestimation of total predicted flows, equal to -3% and -4% respectively, but this time the Final budget is equal to zero for both catchments. The plot of the flow hydrographs (Fig. 5.10) confirms that the model is very accurately predicting most of the event. Only for the early observed flood peak on 19th July is the model underpredicting the flows. From an examination of the SBAR curve in Fig. 5.6 it would appear that only from this event onward are the catchment average SBAR values consistently less than 0.04 m.

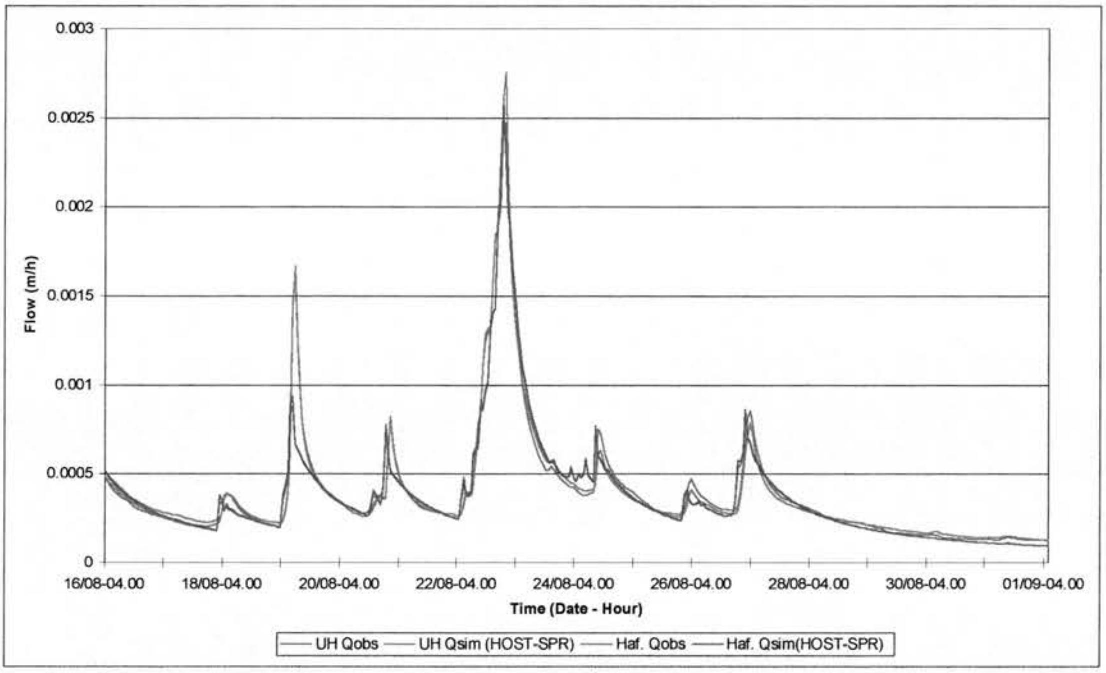

Figure 5.10 – Hydrographs for Event 4

Having examined the simulation results for all four events, there are various observations which can be made. The most obvious one regards the similarity, for both catchments and for all the events, in the results obtained with constant K_0 and HOST SPR K_0 distribution. The differences in model efficiencies and flow component percentages were of the same order of magnitude as those found for the full year simulations. Furthermore, the results for the Upper Hore did not appear to be consistently different from those of the Hafren. We should remember that the Upper Hore was chosen because it was deemed small enough to present, compared to the Hafren, less variation in the topographic characteristics and this would have made the soil-topographic index more sensitive to spatially variable K_0. In reality, the variability of the physical characteristics of the Upper Hore was still comparable to that of the

Hafren, both in terms of soil types and topography. It is therefore not surprising that the Upper Hore results are not significantly different from those of the Hafren.
With regard to the catchment average soil moisture deficit (SBAR) values, there does appear to be a link between TOPMODEL's ability to match observed flows and the existence of a threshold SBAR value (approximately 0.04 – 0.05 m) which is characteristic of the onset of saturation excess flows for the catchment as a whole. We shall explore this aspect in more detail in the following section.

The above results also confirm the importance of the simulated baseflow component as the predominant contributing factor even during flood events. We should note that TOPMODEL's definition of baseflow should not be taken to reflect the actual breakdown of flow components within the catchment. TOPMODEL's baseflow can include what is often referred to as "piston-flow" (Robson et al., 1993; Foster et al., 1997). This latter type of flow occurs when the soil saturated zone exhibits a continuous connectivity throughout the catchment, so that any water input in any part of the catchment is instantly transmitted to the outflow through the saturated zone. Consequently, in the presence of near-surface saturation the model will still attribute to the baseflow component flow which may actually be occuring as near-surface lateral runoff. This would appear to be the only explanation to account for such high percentages of baseflow even for single event simulations.
To conclude, we can state that of all four chosen events, the last one shows the best match over an extended period of time (~ two weeks) covering multiple flood peaks. This could be due to the fact that for earlier events:

- the soil saturated stores in the catchment exhibited a variable degree of spatial connectivity, so that locally generated runoff was not always instantly transmitted to the outflow;
- the retention of water by the peat soils was delaying the catchment response.

But because of TOPMODEL's assumptions of instant transfer of runoff and permanent connectivity of saturated zones, the earlier events show an initially overestimated simulated response which anticipates the measured flows. This is exemplified by Event 2 where the simulated flows are initially greater than the observed flows. Once the connectivity is re-established and the peat soils are nearing saturation, the observed flows then increase significantly - as at the end of Event 2 and for Event 3 – but TOPMODEL does not have sufficient stored volumes to release.

5.3 Simulations of Soil Moisture Deficit

In carrying out the calculation of soil moisture deficit for the Hafren, it was hoped to obtain a better understanding regarding the impact of spatially variable K_0 on the dynamics with which saturated runoff generating areas varied during flood events. The results obtained are examined below in relation to three different aspects.

1) Comparison of SMD maps obtained with the constant K_0 and HOST-SPR K_0. This is in order to highlight any obvious spatial differences between the two distributions of soil lateral saturated conductivity (K_0), as well as describing the SMD patterns during the wetting up and drying down sequence.
2) Quantitative analysis of SMD difference maps obtained by subtracting the constant K_0 SMD from the HOST-SPR SMD maps. This is in order to highlight any temporal variations between the two distributions and within each of the soil types.
3) Comparison of SMD maps obtained for the HOST-SPR K_0 in the vicinity of the assumed SBAR threshold identified for the four flood events. This would clarify whether a characteristic catchment SBAR threshold exists and if it affects the expansion of the saturated contributing areas.

To facilitate the reader, the Hafren soils and the soil-topographic index have been reproduced in Fig. 5.11.

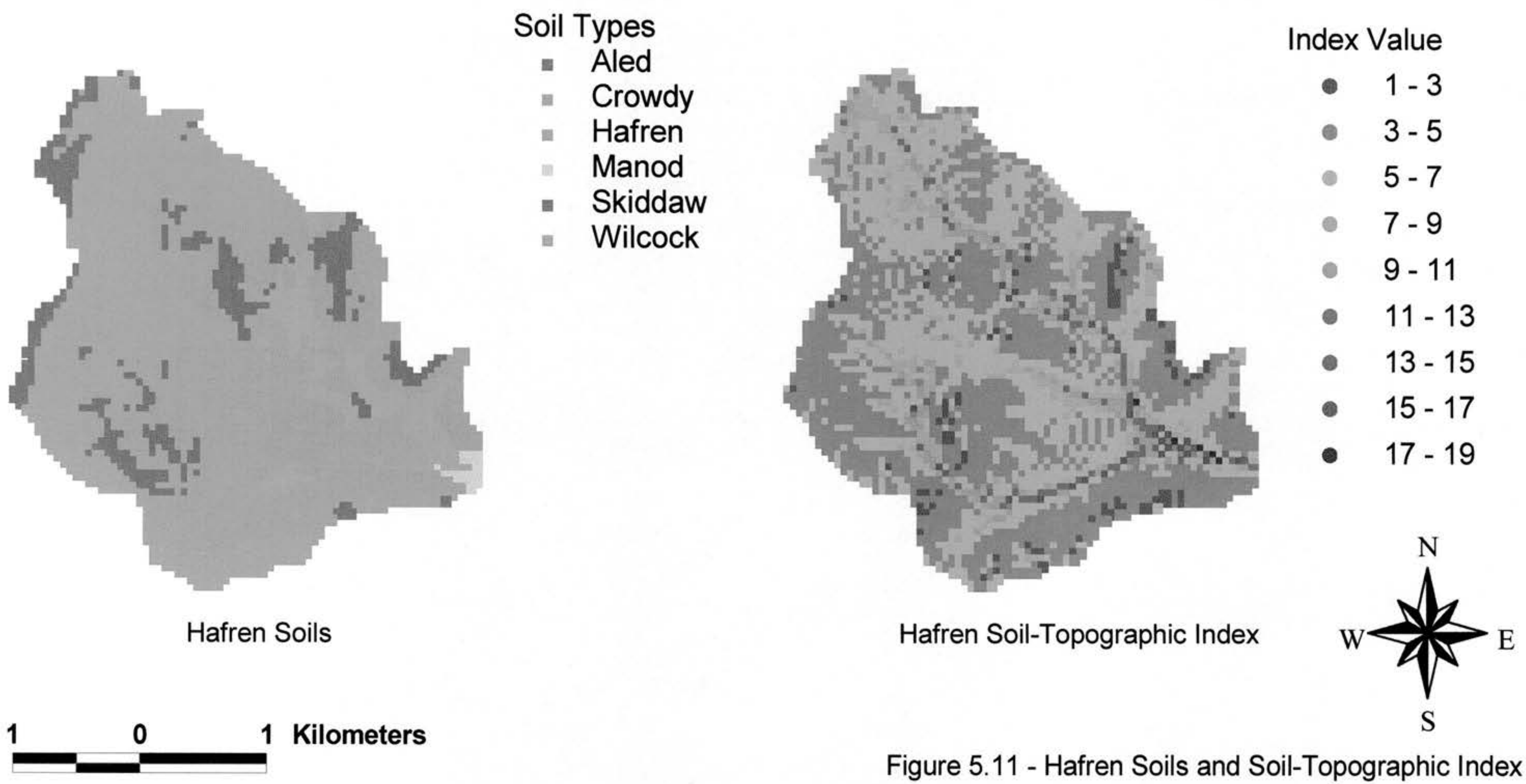

Figure 5.11 - Hafren Soils and Soil-Topographic Index

5.3.1 Qualitative Comparison of SMD maps of the Hafren: Spatially distributed HOST-SPR K_0 vs. Constant K_0

The timesteps chosen for the calculation of the SMD maps (Tab. 5.11) were intended to represent the variations in catchment soil moisture during the wetting up and subsequent drainage phases of the single events. The following paragraphs will therefore examine the various phases separately, by referring to timesteps within each of the four events. It should be underlined that the order in which the different maps will be referred to will reflect a progressive increase or decrease in SBAR, rather than the temporal succession.

Event ID	Timestep (hrs - date)	Hafren Avg. SBAR (m)	Description of Hydrograph Point
E1-T1	3877 - 10/6	$3.36*10^{-2}$	Beginning of rising limb of hydrograph
E1-T2	3887 - 10/6	$5.31*10^{-3}$	Maximum flood peak for 1985
E1-T3	4099 - 19/6	$5.76*10^{-2}$	Last point on hydrograph recession.
E2-T1	4598 - 10/7	$6.25*10^{-2}$	Beginning of rising limb of hydrograph
E2-T2	4617 - 11/7	$2.60*10^{-2}$	Intermediate flood peak.
E2-T3	4657 - 13/7	$3.59*10^{-2}$	Intermediate flood minimum
E2-T4	4659 - 13/7	$2.72*10^{-2}$	Maximum flood peak.
E2-T5	4744 - 14/7	$4.45*10^{-2}$	Intermediate flood minimum
E2-T6	4749 - 16/7	$3.44*10^{-2}$	Intermediate flood peak
E3-T1	4847 - 20/7	$5.08*10^{-2}$	Beginning of rising limb of hydrograph
E3-T2	4858 - 21/7	$3.12*10^{-2}$	Maximum flood peak
E3-T3	4890 - 22/7	$4.09*10^{-2}$	Intermediate point on hydrograph recession.
E4-T1	5551 - 19/8	$4.23*10^{-2}$	Beginning of rising limb of hydrograph
E4-T2	5556 - 19/8	$2.63*10^{-2}$	Intermediate flood peak.
E4-T3	5642 - 23/8	$1.18*10^{-2}$	Maximum flood peak
E4-T4	5650 - 24/8	$2.09*10^{-2}$	Intermediate point on hydrograph recession

Table 5.11 – Timesteps of Soil Moisture Deficit Simulations

At drained conditions the hillslopes and peat areas throughout the catchment usually show SMD values greater than 0.05 m, whereas the peat areas in the northern end and the near-riparian areas generally exhibit the entire range of SMD variability (see Fig. 5.12a)[4]. From a visual comparison between the constant K_0 and the HOST SPR K_0 we can see that:

a) the connected saturated areas coincide with the riparian areas, regardless of the K_0 distribution used;
b) there does not appear to be any significant difference in the spatial distribution of SMD values throughout the catchment, calculated with the two K_0 distributions.

As the catchment begins to wet up, the extent of saturated area increases with the near-riparian areas, the topographic hollows and the peat areas in the northern section being the first to show a significant decrease in SMD (see Fig. 5.12b). These areas are then followed progressively by the hillslopes throughout the catchment and the peat areas at the northern end of the catchment (see Figs. 5.12c,d). At this stage many of the ridges and steeper slopes in the central, east and southern part of the catchment are still quite dry (SMD > 0.05m). Again though, we can clearly see how there are no significant differences between the constant K_0 and the HOST SPR K_0 versions of the soil moisture maps.

With the flows nearing the maximum flood peaks the riparian saturated areas continue to expand up the hillslopes and progressively form a connected drainage network that extends to the catchment boundary (see Figs. 5.12e,f,g). The peat areas to the north of the catchment become almost entirely saturated, while those in the vicinity of Plynlimon summit remain somewhat drier. The ridges and hilltops in the central, southern and eastern part of the catchment still show the highest SMD values. As for the earlier phases of the events, there is no difference between the constant K_0 and the HOST SPR K_0 soil moisture maps.

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[4] Given the difficulty for the reader in visualising the large number of SMD maps in Appendix 2, only the more representative ones will be used to support the observations made in the present section..

In the drainage phase associated with the recession limb the steeper hillslopes and the peat areas near the Plynlimon summit are the first to exhibit a rapid decrease in SMD (see Figs. 5.12h,i,j). These are then followed by the lower hillslope areas and the peat areas to the north of the catchment, with only the saturated riparian areas remaining as the connected drainage network. This behaviour is observed in both the constant K_0 and the HOST SPR K_0 soil moisture maps.

Considering these results with regards to TOPMODEL's description of runoff generating processes, the small length of time that the blanket peats are predicted as being saturated or near-saturated explains the errors in the simulated flows. In particular, the simulations for Event 2 and Event 3 can be taken as examples. The excessively high calculated flows in the early phases of Event 2 are followed by the underestimation of observed flows in the later phases of Event 2 and in Event 3. The above findings are therefore consistent with the hypothesis that TOPMODEL is transforming into runoff a volume of water that is actually stored in the hilltop peats, and then released with a certain delay.

Finally, with regard to the lack of any significant difference between the constant K_0 and HOST SPR K_0 maps, this simply reaffirms the fact that topography is the dominant factor controlling the variability of SMD throughout the catchment. This is confirmed by the fact that the steeper hillslopes with small upslope contributing areas are always the driest, regardless of the soil classification used. From the equation of the soil-topographic index ($\ln(a/T_0*\tan\beta)$) we can see how the small contributing area and high slopes lead to very small index values, and therefore a reduced likelihood of saturation. In the following section we will go on to examine whether there is any relationship between the spatial differences and the different soil types.

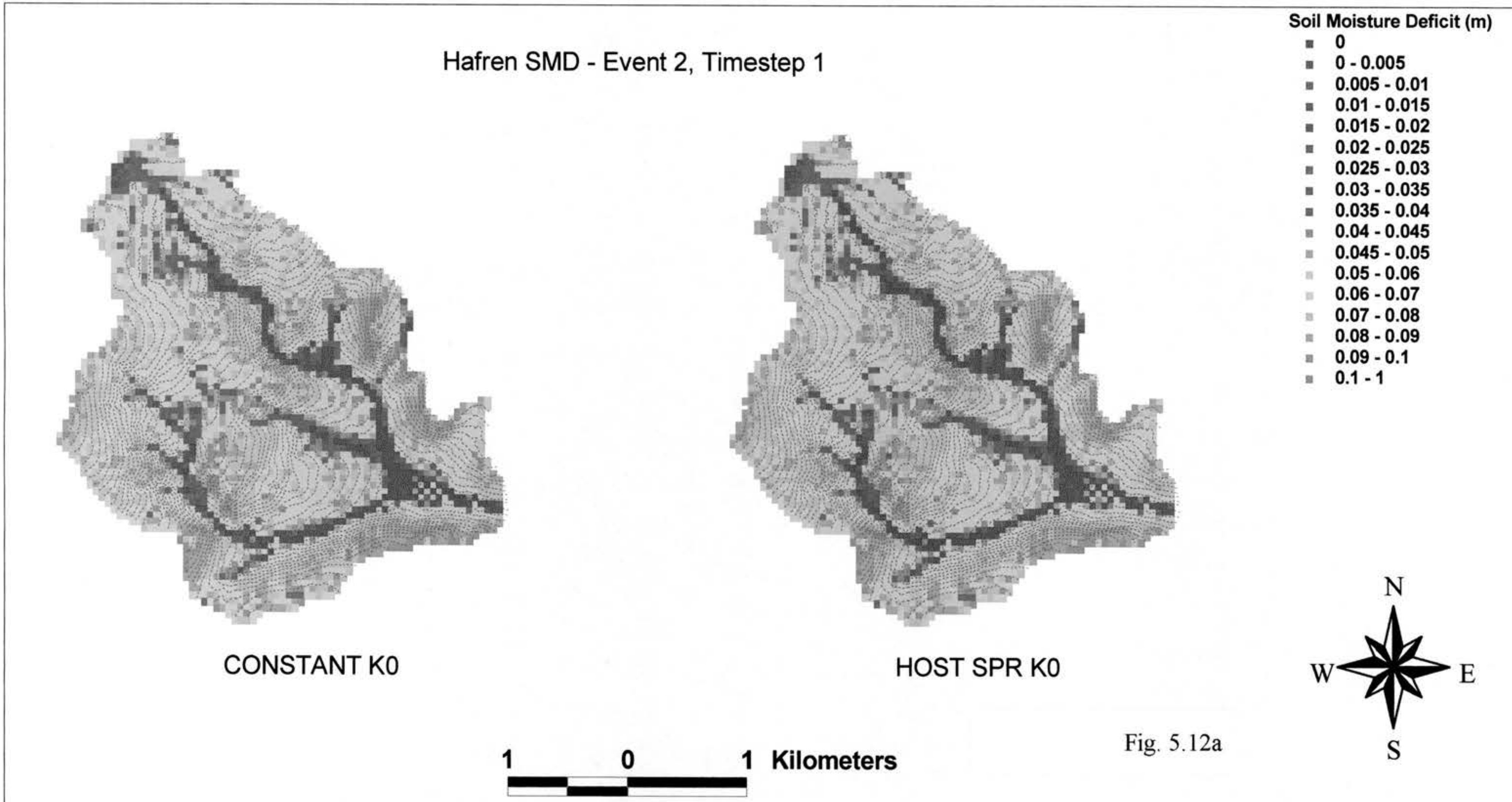
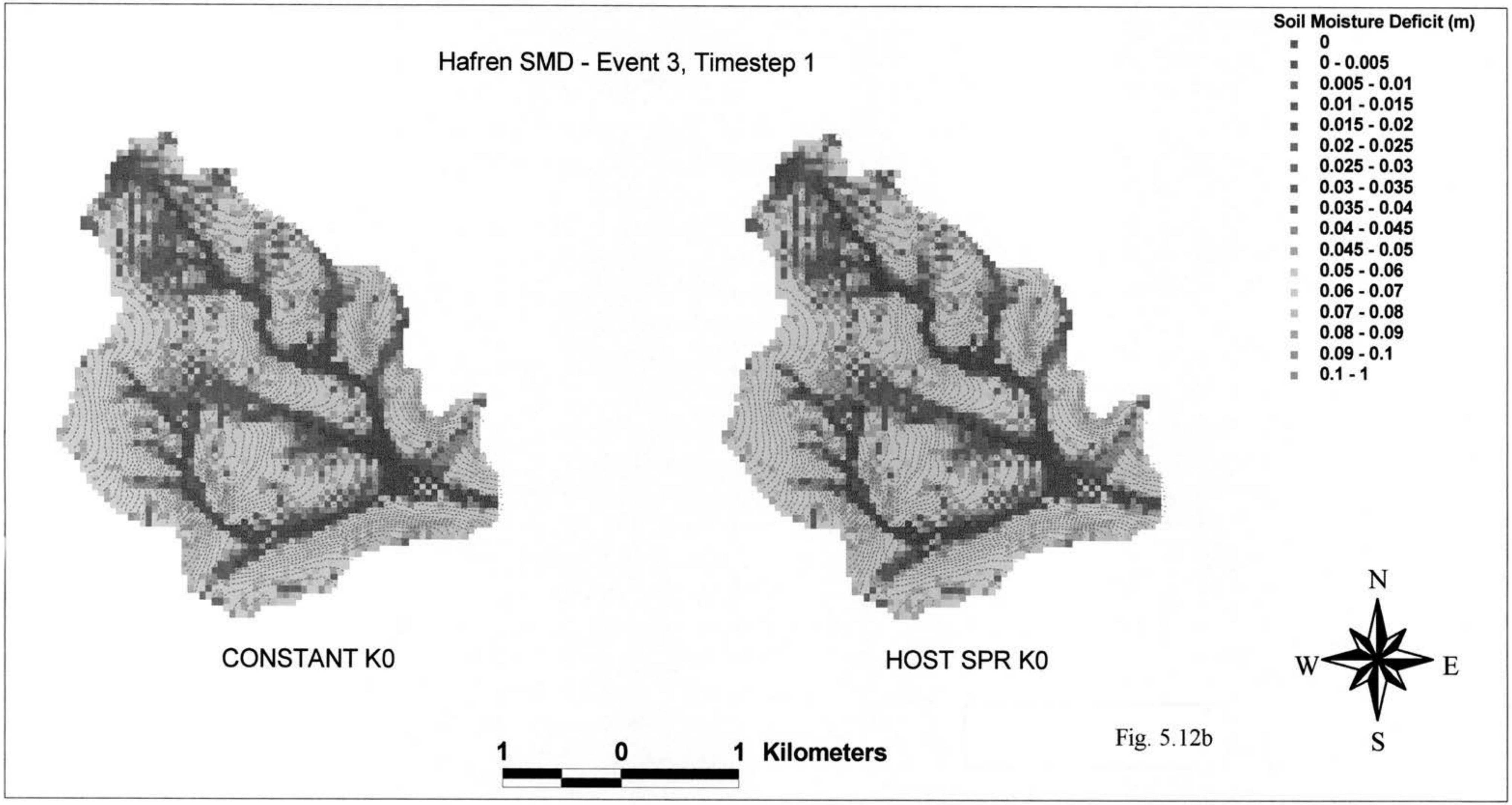

Hafren SMD - Event 2, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
1 0 1 Kilometers
N
W
E
S

Fig. 5.12a



Hafren SMD - Event 3, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
1 0 1 Kilometers
N
W
E
S

Fig. 5.12b

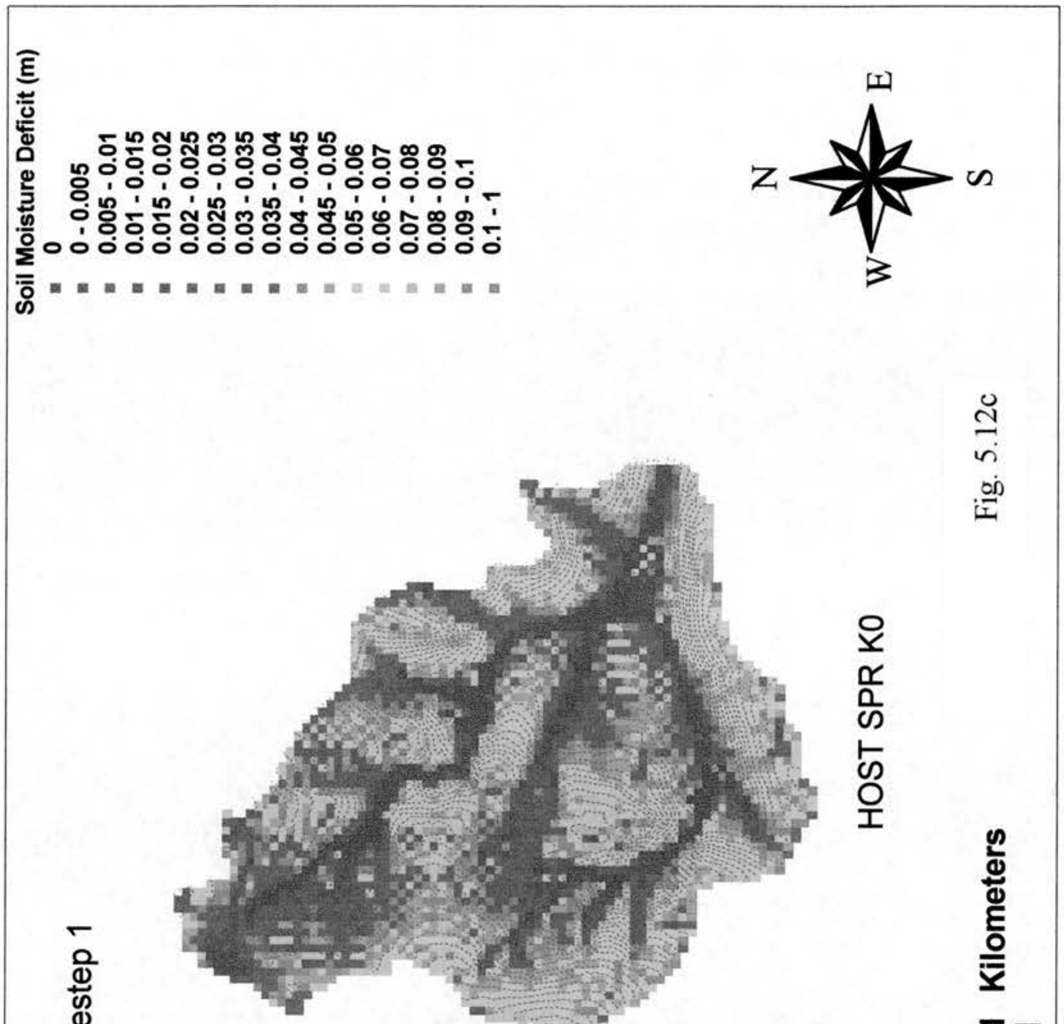

Hafren SMD - Event 4, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
1 0 1 Kilometers
N
E
S
W

Fig. 5.12c

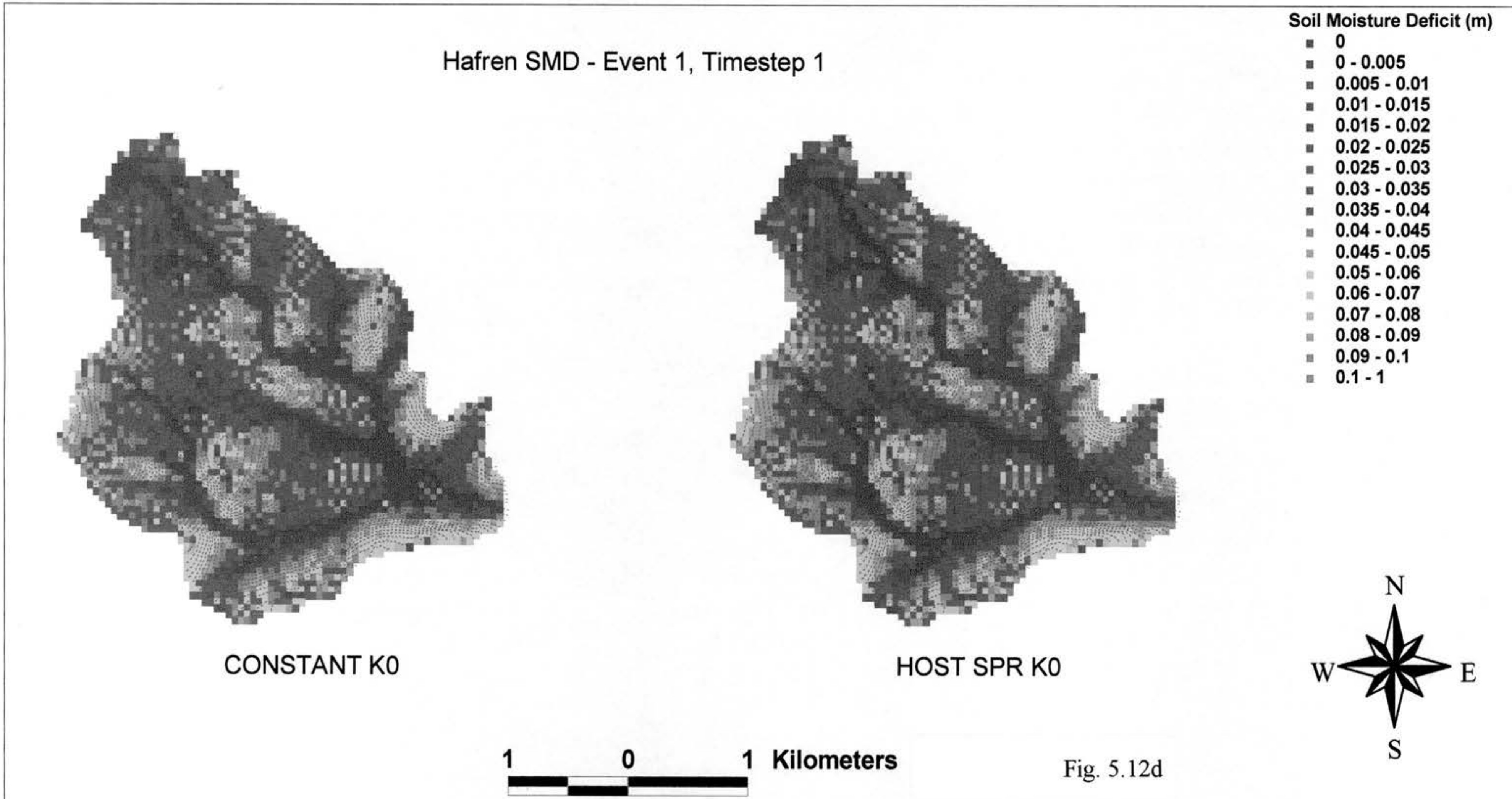
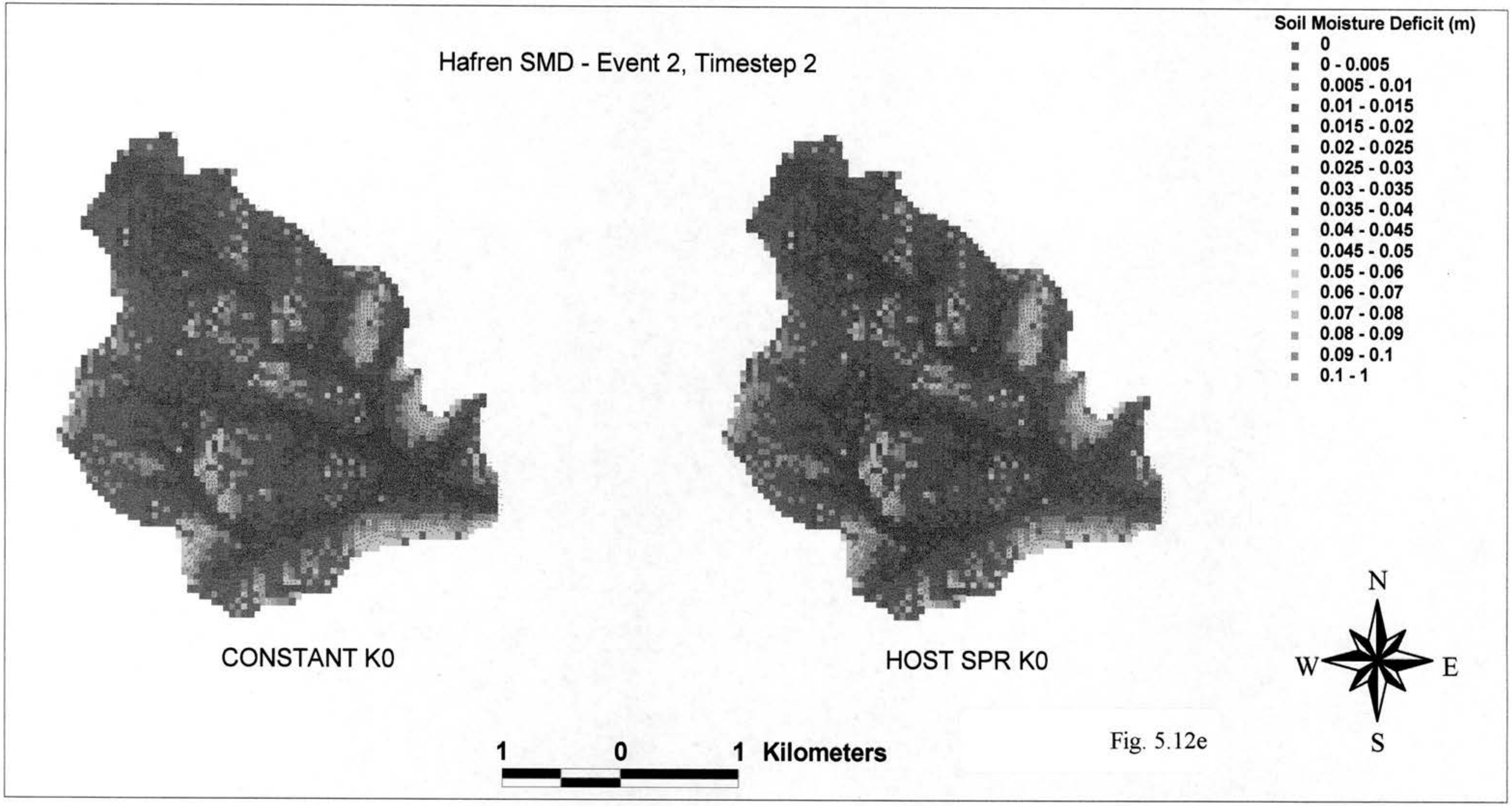
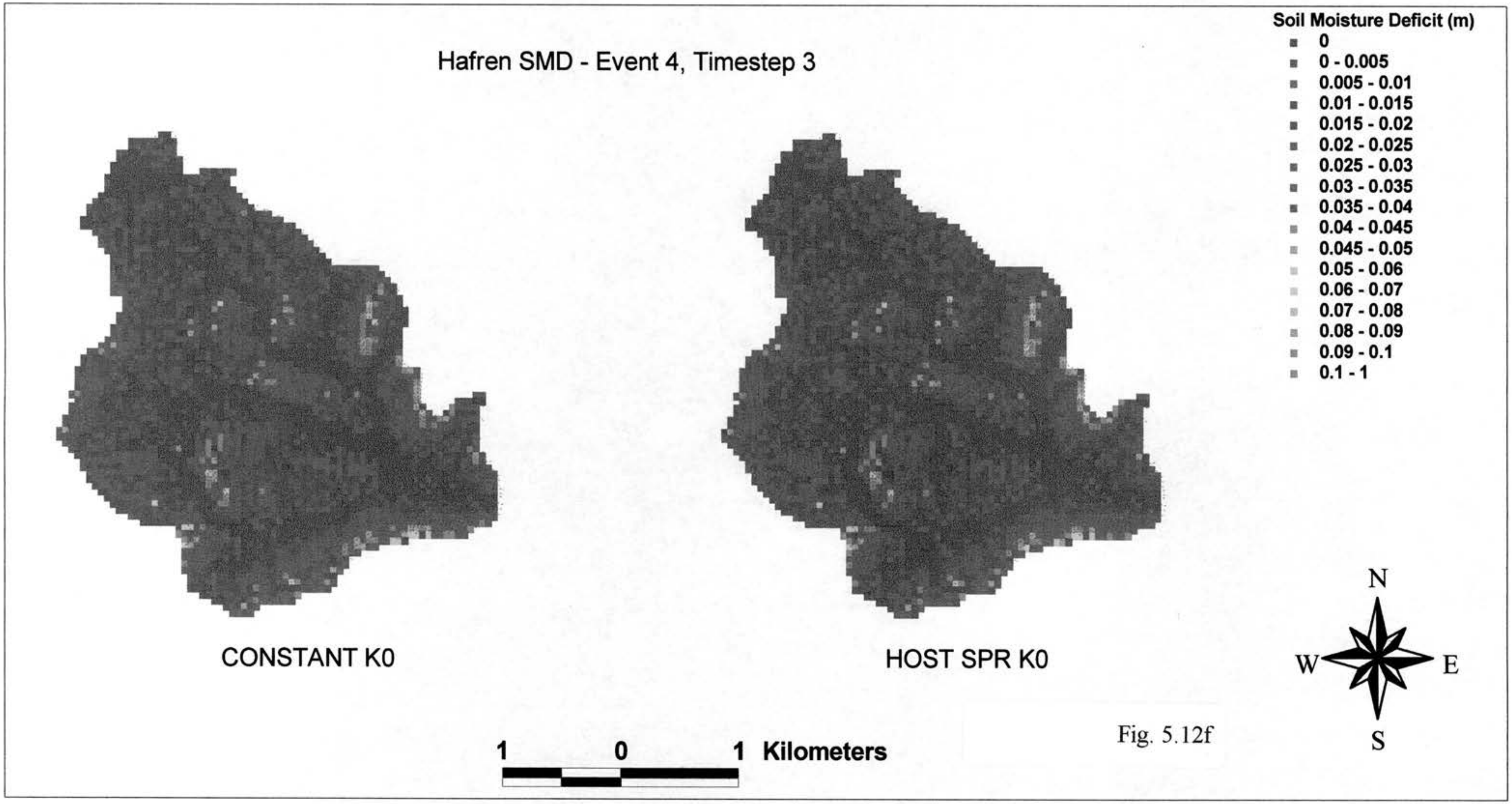

Hafren SMD - Event 1, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

Fig. 5.12d



Hafren SMD - Event 2, Timestep 2
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1 0 1 Kilometers

Fig. 5.12e



Hafren SMD - Event 4, Timestep 3
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
1 0 1 Kilometers
N
W
E
S

Fig. 5.12f

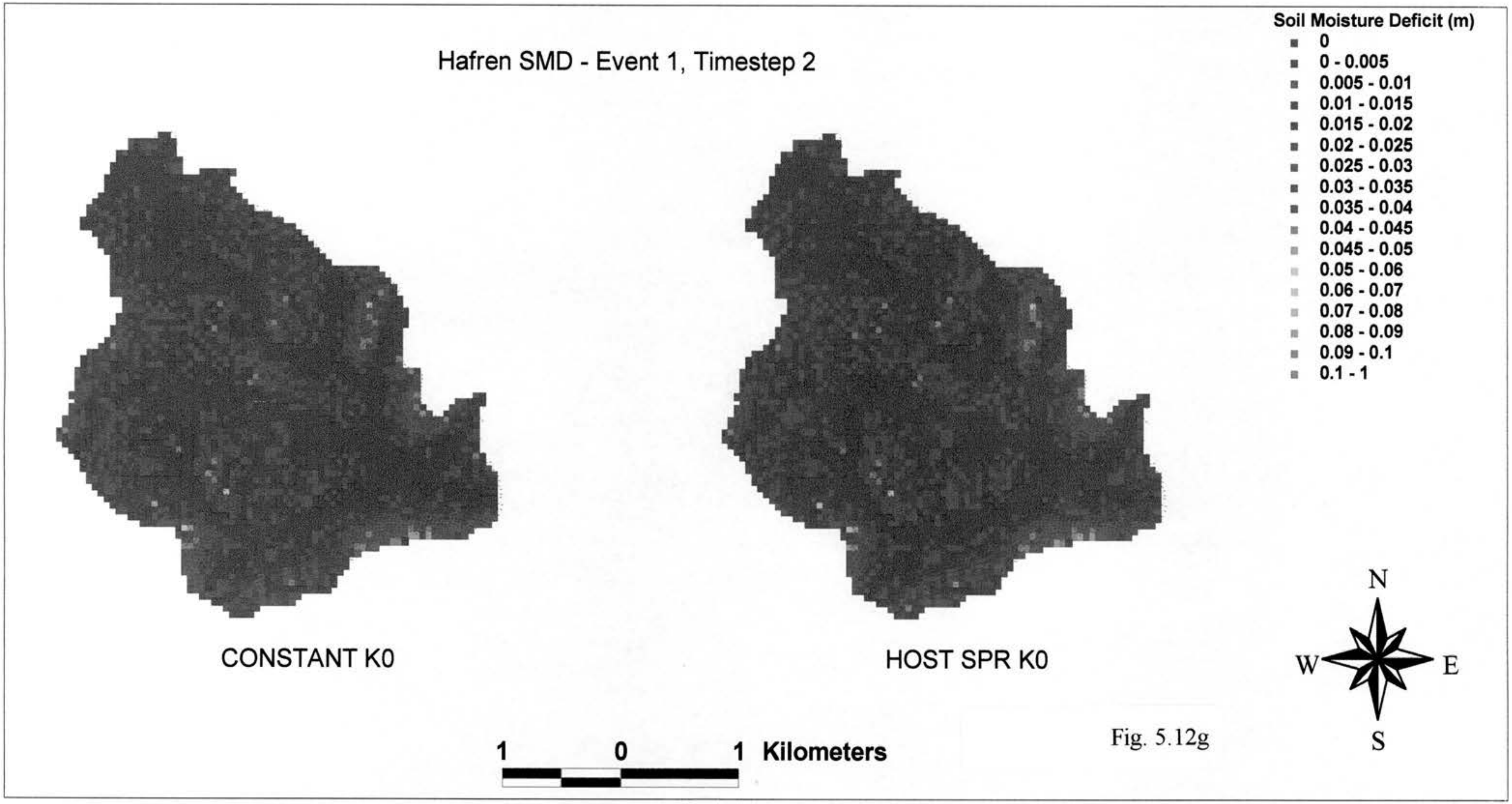

Hafren SMD - Event 1, Timestep 2
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

Fig. 5.12g

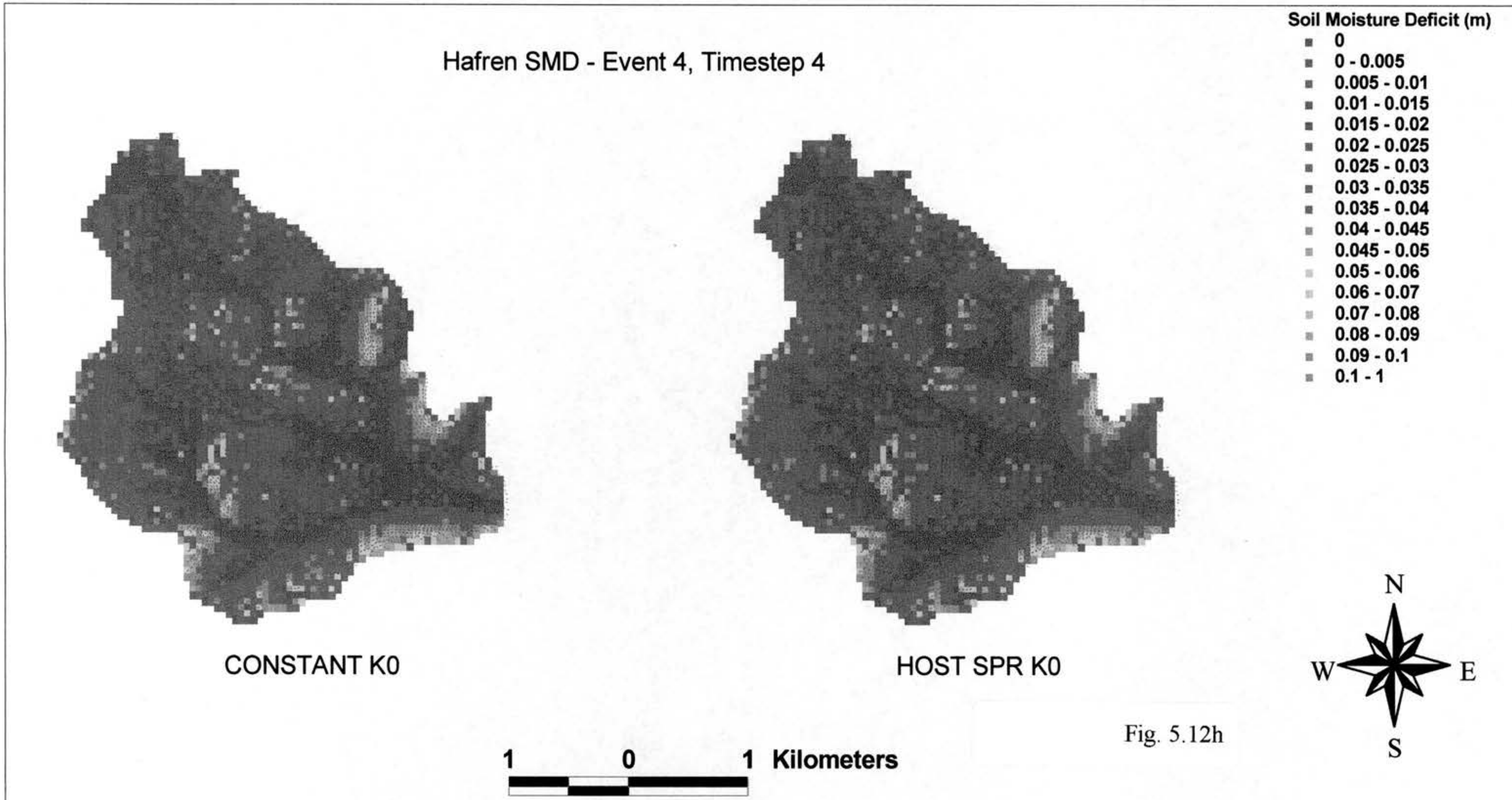

Hafren SMD - Event 4, Timestep 4
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

Fig. 5.12h

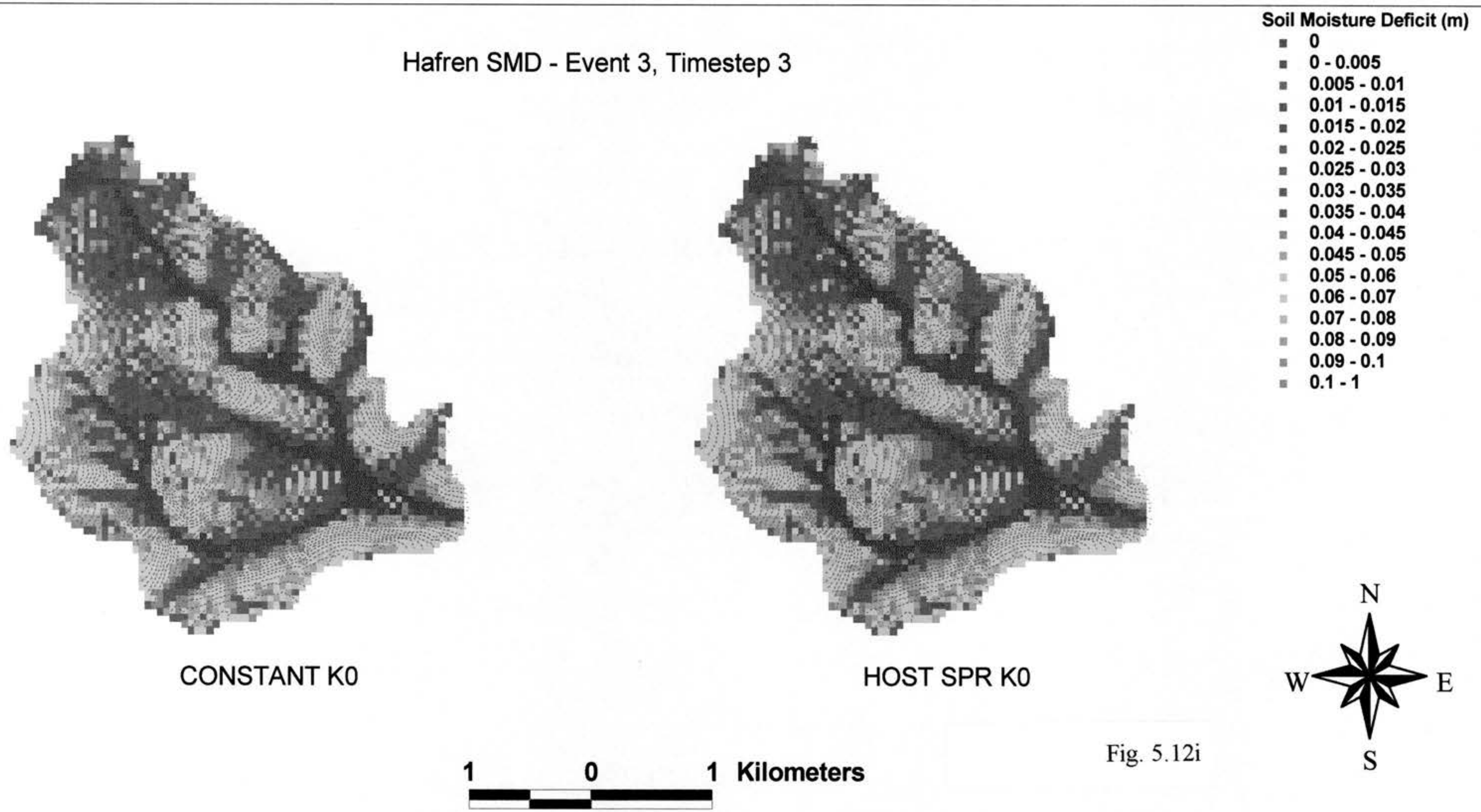
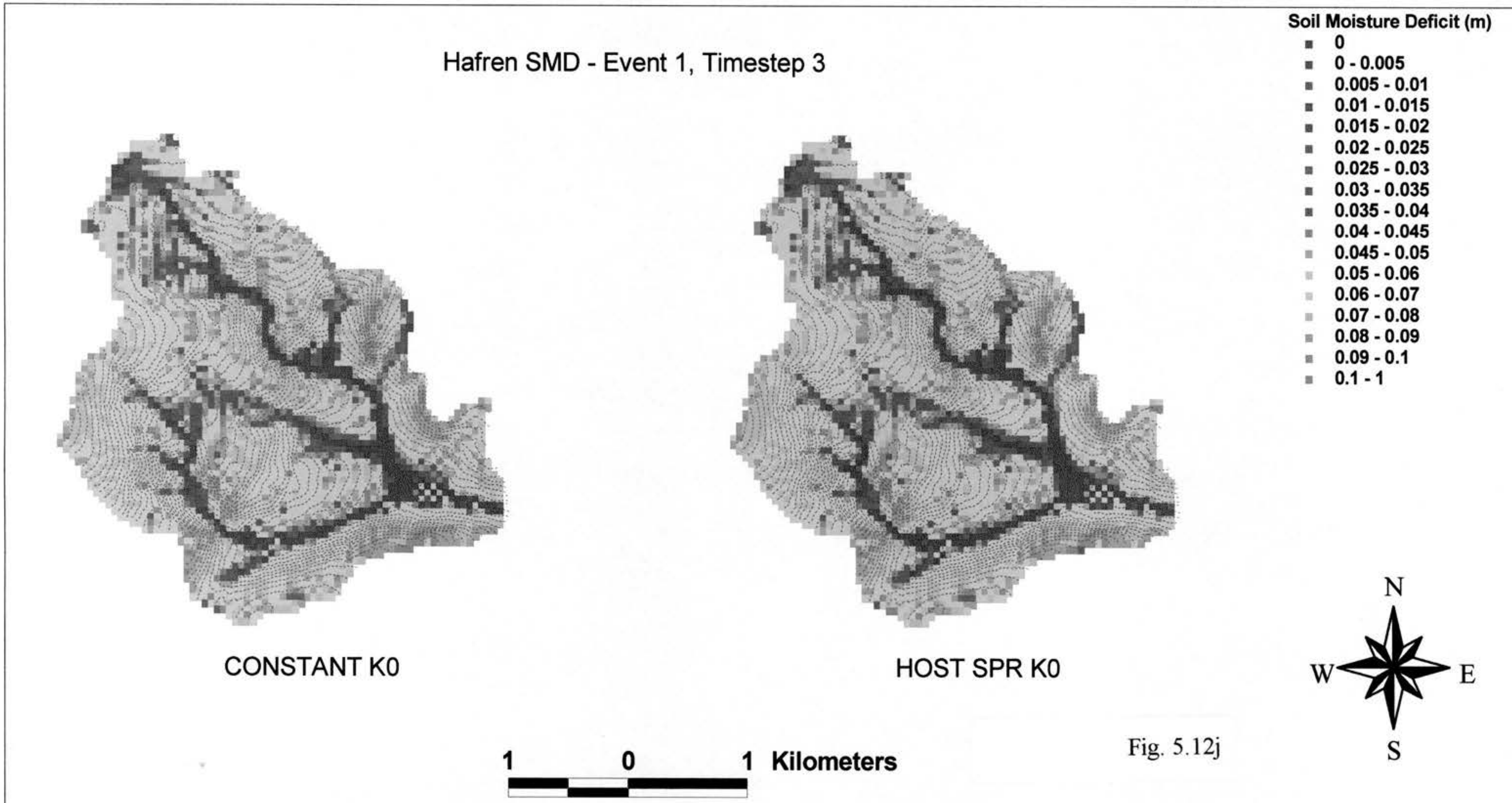

Hafren SMD - Event 3, Timestep 3
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1 Kilometers

Fig. 5.12i



Hafren SMD - Event 1, Timestep 3
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

Fig. 5.12j

5.3.2 Quantitative analysis of SMD differences between the HOST-SPR distributed K_0 and Constant K_0.

The results of the previous section have highlighted the difficulty in identifying significant differences between the constant K_0 and the HOST SPR K_0 maps of SMD. Also, it is difficult to understand the temporal evolution of such differences from a discrete series of snapshots.

For this reason, the quantitative analysis previously described in Section 4.7.1 was carried out, from which several observations and conclusions may be drawn. We should remember that the SMD difference was obtained by subtracting the constant K_0 SMD values from the HOST-SPR K_0 SMD values on a cell by cell basis, and that the SMD values are always positive or zero. The following points will refer to Fig. 5.13, 5.14, 5.15, 5.16.

1) For all of the events the total SMD difference shows negative values except in the vicinity of observed flood peaks. This therefore implies that the during the low and medium flows, the SMD values associated with HOST-SPR K_0 are smaller than those associated with constant K_0. As a result, the HOST-SPR K_0 is predicting more saturated soil conditions over the entire catchment at low and medium flows.

2) Following from the preceding observation, we can state that the positive total SMD difference near the flood peaks for all events indicates that the values of SMD for the HOST-SPR K_0 distribution are greater than the SMD values for the constant K_0 distribution. The model is therefore predicting less saturated soil conditions near the flood peaks over the entire catchment for the HOST-SPR K_0.

3) For events 2, 3 and 4 the total SMD difference presents peaks which slightly anticipate the observed flow peaks by 1-2 hours. This may simply represent a numerical shift between the two SMD distributions attributable to TOPMODEL's algorithms. However, it could also imply that the differences between constant K_0 and HOST-SPR K_0 are more significant in the wetting up phases of the events.

This latter possibility seems confirmed by event 1, where the peak in the SMD difference anticipates the observed flood peak by 7 hours. This implies that, with the HOST-SPR K_0, the model may in some cases respond more slowly to precipitation events, and this would seem consistent with the known water storage properties of the upland peat soils. It is not clear though why this behaviour is not observed for the following three events.

4) For all four events the soils which show the greatest variation in SMD differences over time are the Aled and Manod soils. Both of these soils are generally highly permeable and well drained. For both soils the differences are always less than or equal to zero, and the timing of the peaks essentially reflects the timing of the peaks in total SMD difference. Based on the observations in 1), these results indicate that the HOST-SPR K_0 is predicting more saturated soil conditions for these two soils. This result does not, at first, appear consistent with the nature of the soils, which are not characterised by their ability to accumulate and store water and do not have as great a storage potential as the peat soils. If we consider the HOST SPR index values for these soils (Tab. 4.1) we find that they are equal to 25 and 29 respectively, which are much lower than the area weighted average of 56, and this results in scaled K_0 values of 401 m/h and 465 m/h (Tab. 4.7). With respect to the spatially constant calibrated K_0avg value of 890.798 m/h, the two soils are showing scaled K_0 values which are much lower and this, together with the reduced storage capacity, will result in a much higher likelihood of saturation.

5) Over all four events the differences in SMD are essentially constant for the Crowdy, Hafren, Skiddaw and Wilcock soils. All of the soils mentioned generally contain a peaty layer, whether near the surface (Hafren, Skiddaw and Wilcock) or throughout the entire soil profile (Crowdy). The positive difference values for the Crowdy, Skiddaw and Wilcock soils imply that the HOST-SPR K_0 is predicting less saturated soil conditions for these three soils, and this also is contrary to the expected behaviour of the soils. Instead, the negative values for the Hafren soil type implies that the HOST-SPR K_0 is predicting more saturated soil conditions for these soils. Given the similarity between the Crowdy and the Hafren soils, this

different behaviour is surprising. Yet if we go back and consider the HOST SPR index values for these soils (Tab. 4.1) we find that they are equal to 60 and 48, and are respectively higher and lower than the area weighted SPR average of 56. The above index values result in scaled K_0 values of 962 m/h and 770 m/h (Tab. 4.7). With respect to the spatially constant calibrated K_0avg value of 890.798 m/h, the two soils are therefore showing scaled permeabilities that are higher and lower and this therefore explains the SMD differences predicted by TOPMODEL.

6) Finally, the fact that the SMD differences are essentially constant for all four peaty soil types indicates that for these soils there is no time-dependent effect on the prediction of SMD, as there was for the Aled and Manod soils. This is further proof that TOPMODEL is not able to model the time delay in the storage and release of water by the peaty soils, but rather is assuming a constant behaviour over time.

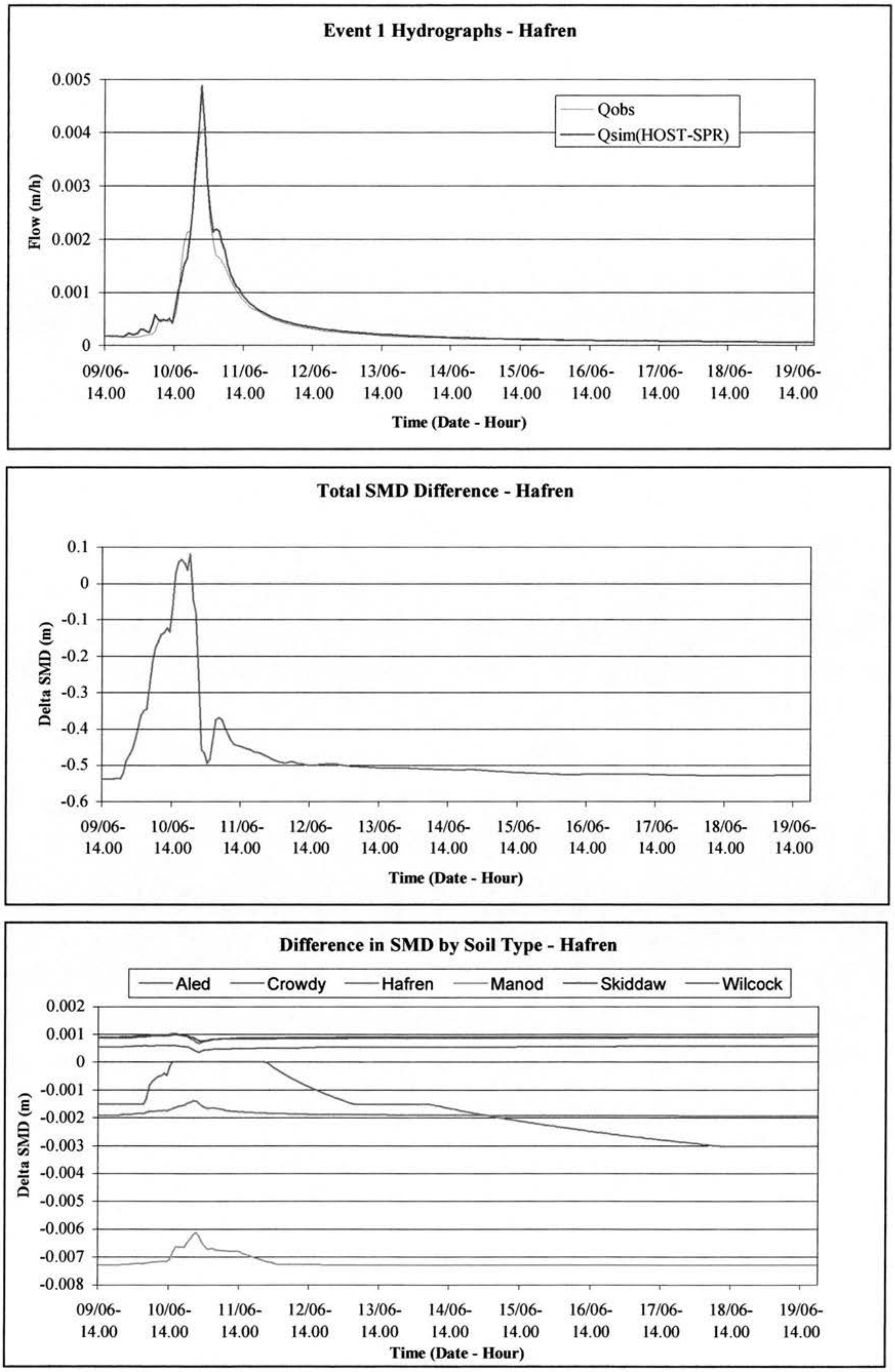
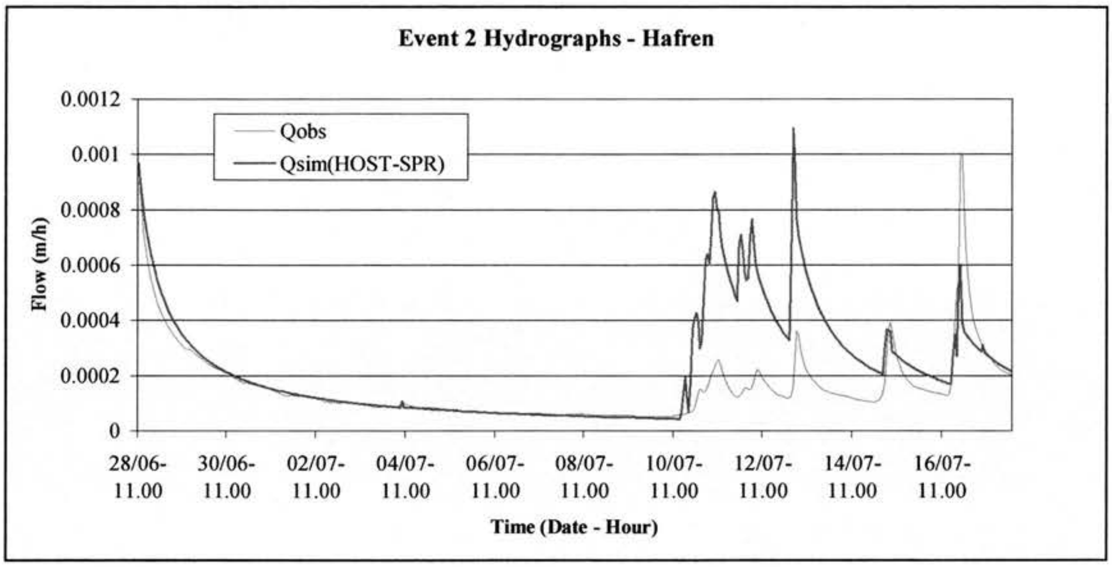
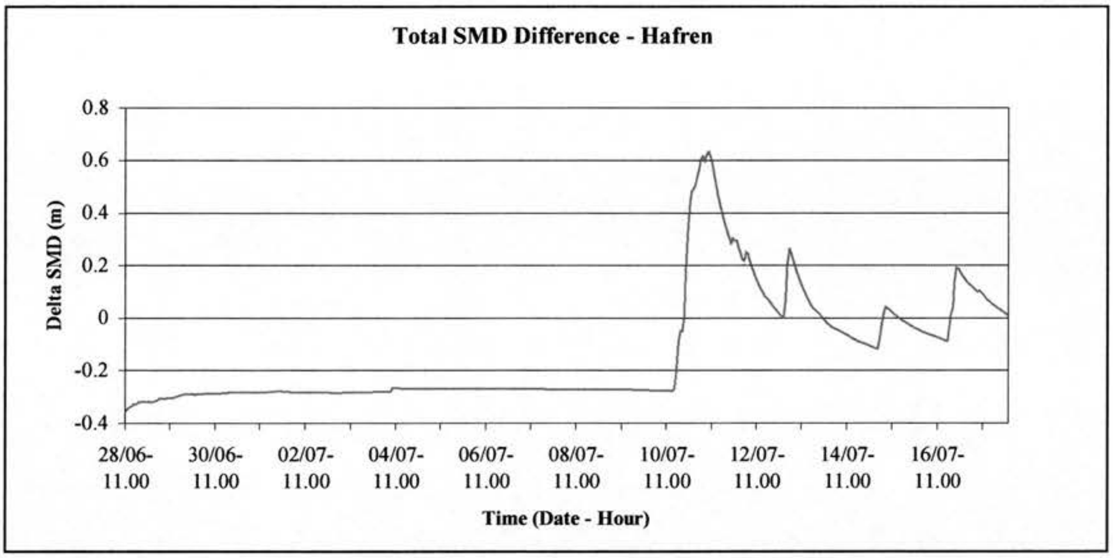


Figure 5.13 – Event 1 SMD Calculations





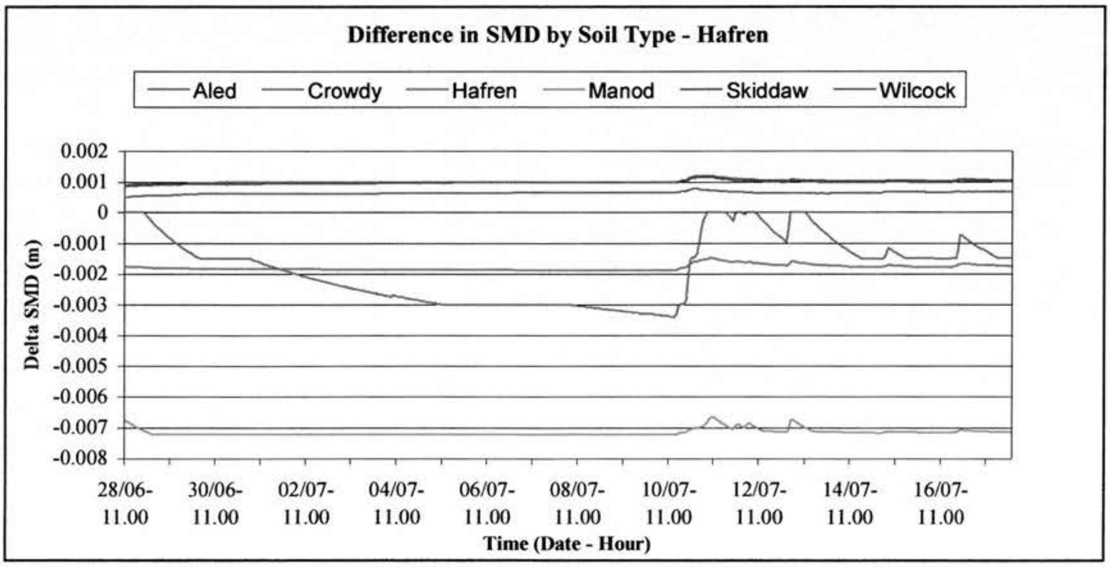


Figure 5.14 – Event 2 SMD Calculations

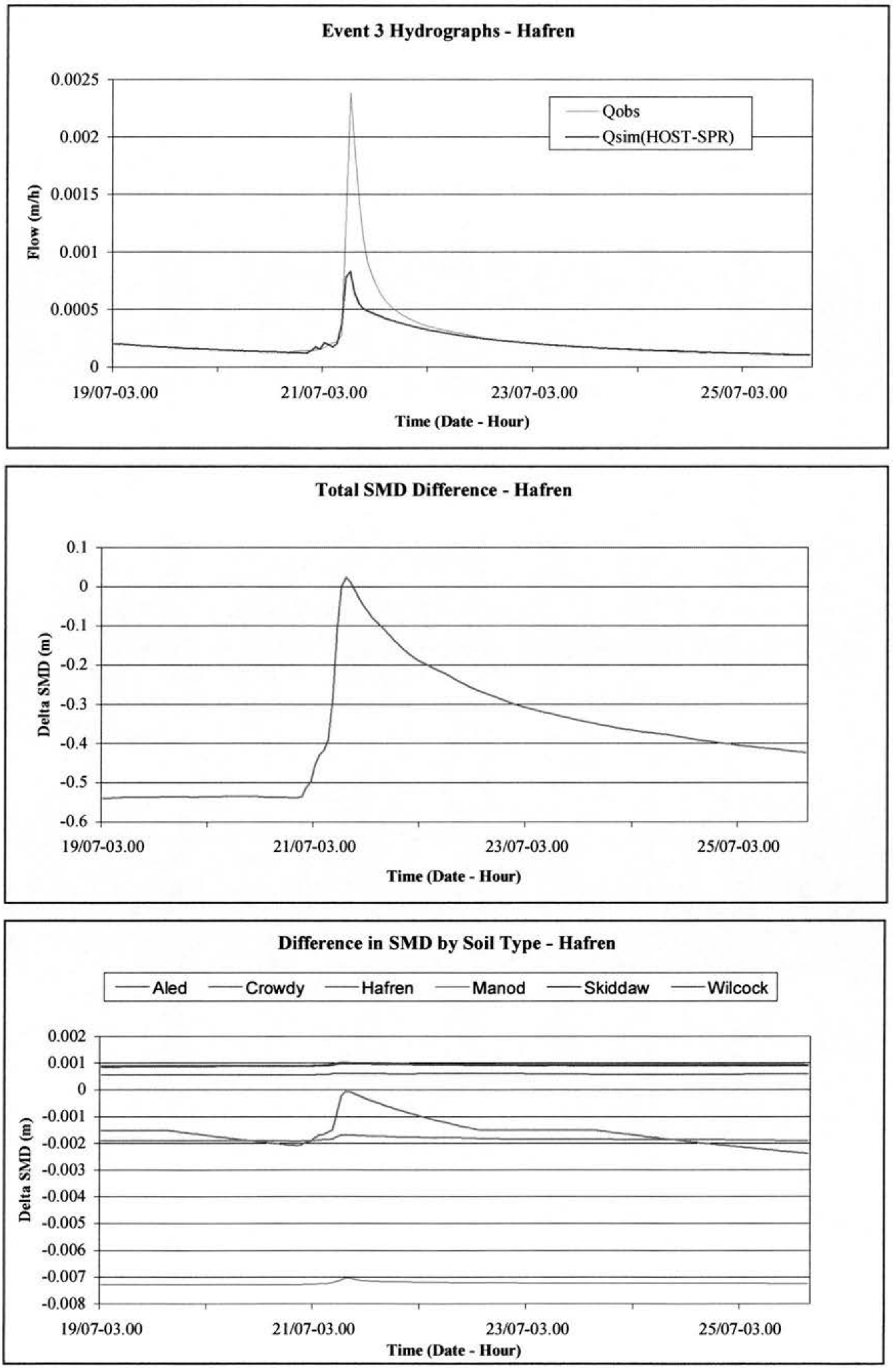


Figure 5.15 – Event 3 SMD Calculations

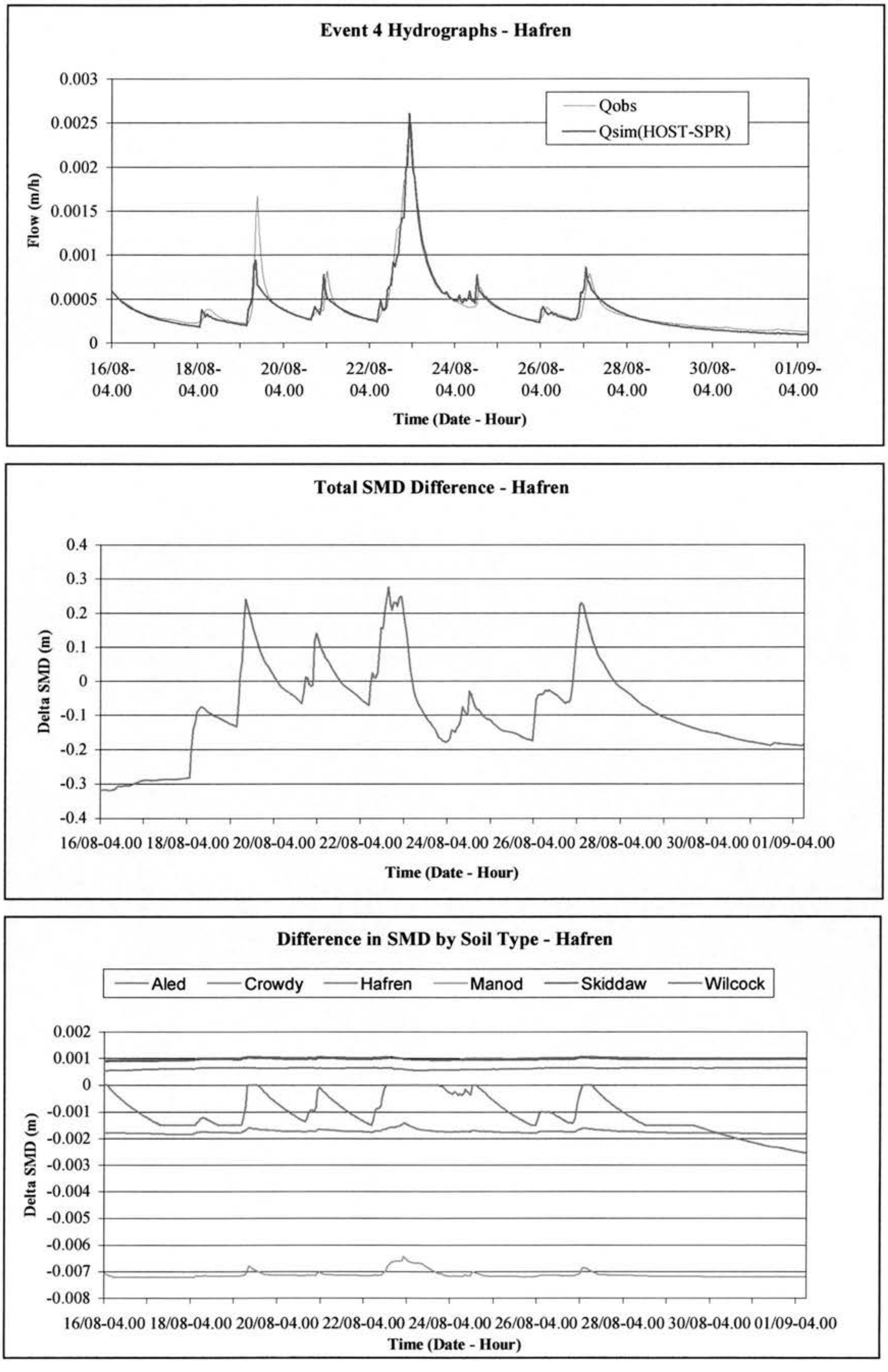


Figure 5.16 – Event 4 SMD Calculations

The above results are also confirmed if we examine the SMD difference maps in Appendix 3[5]. In particular, we can see that:

a) for all four events the maps show negative SMD difference values for the Hafren, Aled and Manod soils and positive SMD difference values for the Crowdy, Skiddaw and Wilcock soils;
b) over the course of the events the magnitude of the differences remains almost constant;
c) over the course of the events the saturated areas are always connected to the permanently saturated near-riparian areas, as already shown in the SMD maps in Section 5.3.1.

Based on the above results we can therefore conclude that considering spatially variable soil properties:

a) does not affect the manner in which TOPMODEL predicts the expansion of the saturated areas;
b) does affect the SMD variations in the different soils compared to the constant K_0 case. In particular, if the scaled K_0 of a soil is greater than the constant K_0avg, then in the spatially variable TOPMODEL simulations the soils' SMD values will be greater than for a constant K_0, and the soil will be drier. Instead, if the scaled K_0 is less than the constant K_0avg, then in the spatially variable TOPMODEL simulations the SMD values will be less than for a constant K_0, and the soil will be wetter. It is as if the scaled HOST SPR K_0 value is acting as a combined index of soil saturated conductivity (K_0) and soil saturated zone storage capacity, so that soils with scaled K_0 above K_0avg have a larger capacity and therefore are less likely to saturate. On the other hand soils with scaled K_0 below K_0avg have a smaller capacity and therefore are more likely to saturate. We shall return to this aspect in Section 5.3.4.

---

[5] To maximise the visual effect of the differences, they have been plotted with respect to the standard deviation. Also, it should be noted that all blank cells within the catchment are those with predicted SMD = 0 for both constant K0 and HOST-SPR K0.

5.3.3 Qualitative Comparison of SMD maps of the Hafren: Does a Threshold SBAR Exist?

The simulated SMD predictions in the previous sections have highlighted the importance that the hillslopes assume for TOPMODEL, in terms of saturated runoff generating areas. This simulated behaviour though does not correspond to field-based experience of the actual runoff generating processes in the Plynlimon catchments. It is generally believed that apart from the near-riparian saturated areas, runoff generation in the catchment is controlled by the hilltop blanket peats (Roberts and Crane, 1997). These are capable of storing large amounts of precipitation and releasing it very slowly during interstorm periods. This release feeds lateral subsurface flows in the hillslopes and, ultimately, reaches the permanently saturated areas in the valley bottoms. The peats are therefore an important cause of permanent saturation in the near-riparian areas during dry conditions. During storm conditions, the peats accumulate water until – in the presence of sufficient rainfall - they reach near-saturated conditions. Only at that point does surface overland flow begin to manifest itself, though it generally reverts to subsurface lateral flows in the hillslopes. Given that the subsurface flow from the peats and hillslopes is generally greater than the stream outflow, the saturated areas will eventually expand up the hillslopes for the longer duration and/or more intense precipitation events.

The analysis of the single event hydrographs has highlighted TOPMODEL's ability to match observed flows once the catchment SBAR value is less than 0.04 m. It is therefore natural to wonder what occurs to the simulated patterns of SMD in the vicinity of this assumed threshold. In particular, it would be interesting to verify whether below such a value of SBAR the spatially connected low SMD zones extend to include the upland peat soils and, also, how such patterns compare to those near the flood peaks.

In order to shed light on how TOPMODEL actually models the above transitions, it was decided to simulate the variation in SMD over individual timesteps, considering only the HOST SPR results. The timesteps were chosen from individual flood peaks within each of the four events, which satisfied all of the following conditions:

a) initial SBAR > 0.04m;
b) maximum simulated flood flows high enough for extensive saturation to occur;
c) Qsim flows must match Qobs flows very well, otherwise the model is grossly misrepresenting what is happening in the catchment.

Of the four events, only Event 1 matched all three conditions. None of the flood peaks in Event 2 matched conditions b) & c), whereas Event 3 does not match condition c). For Event 4 the flood peaks which were matched very well all had initial SBAR less than or equal to 0.04m. Based on the above considerations, the following timesteps were chosen:

a) Event 1, T=3866 – 3872 to represent the SMD transition through SBAR = 0.04 m;
b) Event 4, T=5636 – 5648 to represent the SMD transition through the flood peak, and compare it to conditions in case a).

The timesteps and associated SBAR values are summarised in Tab. 5.12. The SMD maps for the chosen timesteps are shown in Figs. 5.17 and 5.18.

Beginning with the SMD maps for the Event 1 timesteps, we can observe that:

- only once the SBAR = 0.04m threshold is crossed do the low SMD zones (less than 0.02m) begin to expand up the hillslopes;
- the expansion of saturated areas moves upward and outward from riparian area;
- there do not appear to be any expanding nuclei of areas of low SMD emerging on the upslope peat soils below SBAR = 0.04 m;
- most of the peat soils only start showing decreasing SMD values once the low SMD areas have extended far enough up the hillslopes.

If instead we look at the SMD maps for Event 4, for which the SBAR values are much lower than 0.04m, we notice that:

- extensive saturation of the peat soils to the north of the catchment only occurs near the flood peak conditions, while the peat soils near the Plynlimon summit and in the southern slopes remain noticeably drier even at maximum flood conditions;

- after the flood peak the drainage of peat soils begins immediately and, more importantly, precedes that of the hillslope soils.

Event – Timestep (hrs) & Date, Time	SBAR(m)	Description
E1 – 3866 10/06, 0200	0.0425	Max. SBAR for Event1
E1 – 3869 10/06, 0500	0.0417	-
E1 –3870 10/06, 0600	0.0399	-
E1 – 3872 10/06, 0800	0.0353	-
E4 – 5633 22/08, 1700	0.0265	-
E4 – 5636 22/08, 2000	0.0230	-
E4 – 5642 23/08, 0200	0.0118	Max. Flood Peak for Event4
E4 – 5648 23/08, 0800	0.0187	-

Table 5.12 – Summary of Timesteps for SMD Detailed Simulations

From the above results we can conclude that:

a) the SBAR value of 0.04m may represent a threshold value below which the permanently saturated near-riparian areas start expanding up the hillslopes;

b) TOPMODEL cannot model the emergence of isolated low SMD or saturated areas in the upland peat soils;

c) the peat soils in the higher parts of the catchment only reach saturation or near-saturation values near the flood peaks, and then start draining very quickly immediately after the flood peak.

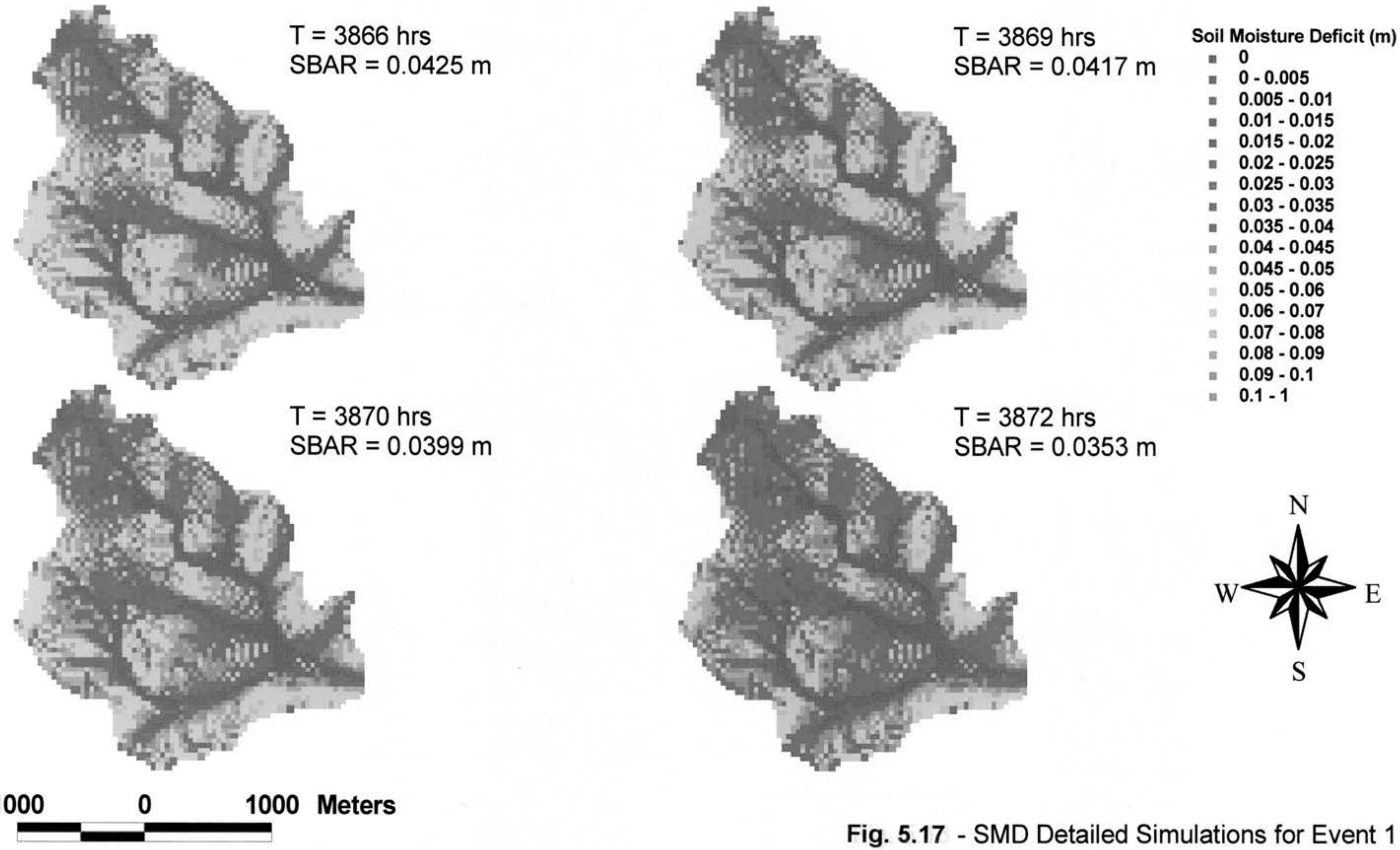


Fig. 5.17 - SMD Detailed Simulations for Event 1

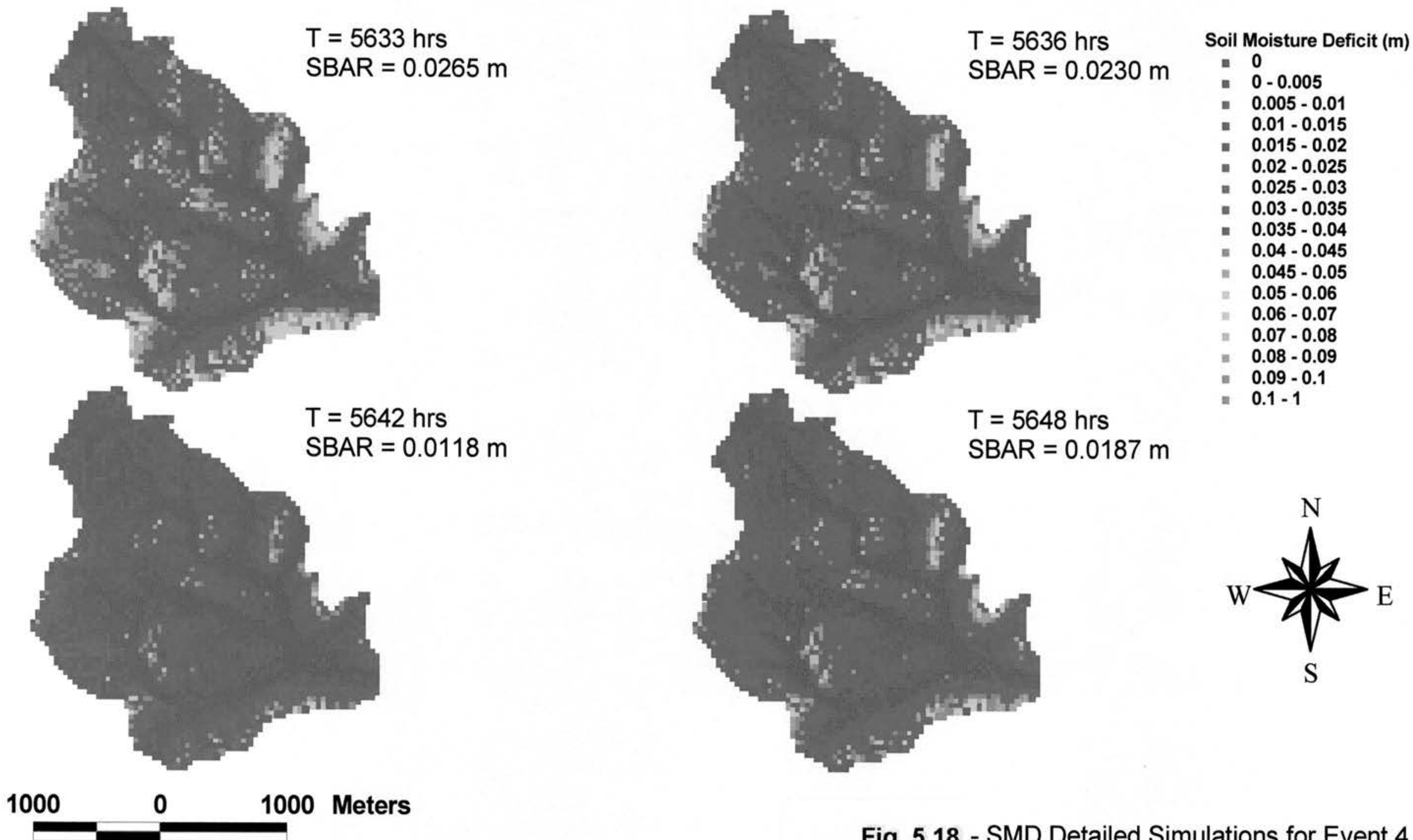


Fig. 5.18 - SMD Detailed Simulations for Event 4

5.3.4 Interpretation of SMD Results

From the results presented in the previous three sections, the picture that emerges may at first appear contradictory. On the one hand the results confirm that:

a) topography is the dominant factor controlling the expansion of saturated areas;
b) the small SMD differences between the HOST SPR K_0 and the constant K_0 can be explained in light of the HOST SPR index values and the storage capacity of the individual soils, though they may appear counter-intuitive from the TOPMODEL perspective;

But on the other hand, the results have also highlighted that the timing of the water storage and release mechanisms in TOPMODEL is not consistent with field experience and with respect to the observed flow generating mechanisms in the catchment, as described by Roberts and Crane (1997). Accordingly, the expansion of the saturated contributing areas in the catchment is not consistent with field-based knowledge of runoff mechanisms in the Plynlimon catchments.

In particular, what appears inconsistent is the representation of the peat's behaviour given that TOPMODEL:

a) does not show any significant response in the SMD of some peat soils until the hillslopes are close to saturation;
b) predicts very rapid draining of the peat soils after the flood event, whereas it is actually the slow release of water by the peats that is an important factor in maintaining the permanently saturated riparian areas.

With regards to the first point, it appears that the K_0 parameter used by TOPMODEL, together with the m and SRMAX parameters, is simply acting as a spatially lumped calibration parameter for the modelling of flows. TOPMODEL is therefore not able to use K_0 to improve the spatial representation of soil moisture deficits.. The fact that none of the published K_0 distributions (LITT.1 and LITT.2) gave sensible results confirms that TOPMODEL is not capable of incorporating physically meaningful K_0 values.

With regards to the second point, the simulation results highlight an important conceptual limit in how TOPMODEL treats the saturated zone within the soil column. Given that the depth of the saturated zone is not specified within the model, this means that the soil moisture deficit is considered an absolute value which has the same effect on runoff generation for all soils. In this manner though, no consideration is given to the actual storage capacity of the saturated zone. We should remember that TOPMODEL always assumes that the rate of variation in the SMD is the same for all soils, because it is controlled by the rate of variation of the catchment average soil moisture deficit (SBAR) in Eqn. 3.9, with the other terms of the equation being constant in time. This conceptualisation of the soils though is contrary to the behaviour of the peat soils within the Plynlimon catchments because:

a) the drainage properties of the Aled and Manod soils are generally much better than those of the peat soils;
b) even if the drainage properties of all the soils were the same, the current understanding on the role of peats in the Plynlimon catchments indicates that their contribution to runoff is controlled more by the remaining volume of water in the saturated zone than by the soil moisture deficit.

Overall, the above problems can therefore be explained by the fact that the soil-topographic index is dominated by the topographic component and is not correctly representing flow processes in the soil saturated zone.

Another aspect to consider is whether the HOST classes do reflect the storage capacity of the individual soils in the Hafren, as the results in Section 5.3.2 seem to imply. Recalling the factors used in defining the HOST classes, the Integrated Air Capacity (IAC) is used as a surrogate for either saturated hydraulic conductivity in permeable soils (Classes 9, 10), or for storage capacity in slowly permeable and impermeable soils (Classes 18-23). With regards to the Hafren catchment, the HOST classes to which the soils belong are listed in Appendix B of Boorman et al. (1995), and are shown in Tab. 5.13.

	Alun[6]	Crowdy	Hafren	Manod	Skiddaw	Wilcocks
HOST SPR	25	60	48	29	60	59
HOST Classes	10	29	15	17	27, 29	26

Table 5.13 – HOST Classes of Hafren Soils

From the table we can see that for none of the Hafren soils does the HOST-SPR index take into account the IAC as a surrogate for the storage capacity of the soils. But the peaty soils do belong to HOST classes (15, 26, 27, 29) for which the flow response model is dominated by the presence of a peaty surface layer, which in turn influences the storage capacity (Boorman et al., 1995). Given the importance of the storage capacity of the peat soils, it would certainly be useful to understand how accurately the HOST index values represent the range of storage capacities within the different peaty soils. This is certainly an area that could be explored in future research. If future work showed that the accuracy was considered satisfactory, we could indirectly account for the soil storage capacity - through the HOST SPR index - even though TOPMODEL does not explicitly consider it in its' representation of the soils.

Finally, we should also note that it is unfortunate that in the case of the Hafren, the catchment is dominated by 4 soil types (Crowdy, Skiddaw, Wilcocks and Hafren) with very similar HOST SPR index and scaled K_0 values, which reduces the range of variability in the SMD predictions. Perhaps a catchment with a more balanced distribution of soils would have shown greater variability, especially in terms of SMD. But in any case, the normalisation of K_0 values has certainly further reduced any variability between the HOST SPR and constant K_0 SMD distributions.

[6] The Aled soils are a subseries of the Alun soil association.

5.4 Conclusions

The principal objectives of the present research were to incorporate spatially variable soil saturated conductivity (K_0) and evaluate TOPMODEL performance:

a) in terms of total catchment or subcatchment outflow over a hydrological year;
b) in terms of prediction of total outflow for single flood events;
c) in terms of the ability to predict soil moisture deficit (SMD) and saturated runoff generating areas.

The methodology adopted has allowed a critical evaluation of the limits of including spatially variable soil data within TOPMODEL. By evaluating a variety of soil classification systems, the present research has also provided insight into the usefulness of such classifications as input to the soil-topographic wetness index used within TOPMODEL.

In particular, the main findings of the research are summarised below.

- The inclusion of a spatially variable K_0 has not led to an improvement in model performance relative to predicted outflow, both at the catchment and subcatchment level.
- The analysis of single flood events confirmed that TOPMODEL's ability to accurately predict catchment outflow was directly related to its' ability to accurately represent the spatial connectivity of contributing areas.
- TOPMODEL's inability to correctly represent the storage – discharge mechanism within the peat soils led to inaccurate estimates of soil moisture deficit and, consequently, of the volume of catchment outflow for some of the individual flood events.
- The use of the spatially distributed HOST Surface Percentage Runoff (SPR) index values did not lead to significantly improved predictions of soil moisture deficit in the different soils. But it did help to underline the primary role of the saturated zone storage capacity when estimating the occurrence of saturation within the individual soils.

Within the scope of a low-level integration with a GIS, the present research has confirmed the main advantages and limits of such an approach. The greater flexibility allowed in data pre-processing and post-processing did not constrain the representation of data and thus facilitated the formulation of questions and doubts on the actual meaning of the model predictions. Yet this in turn also represented the main disadvantage of such an approach: the difficulty in correctly interpreting – and the risk of misinterpreting - spatially distributed model results without an adequate amount of field data to validate and support the model results.

Building on the ideas of Grayson et al. (1993), the interpretation of the results has shown how the combination of simple spatial modelling and qualitative reasoning can lead to a better understanding of the simulated processes and, just as importantly, of the limitations deriving from the input data.

Finally, it is hoped that the results of this research will provide some useful ideas and suggestions on how to tackle related problems within the more application-oriented context of integrated catchment management, specifically in relation to flood prediction, land-use changes and water quality modelling, where the identification of saturated contributing areas and soil moisture deficit plays an important role.

6. Conclusions

The present research has attempted to develop an integrated methodology for the modelling of spatially distributed soil moisture deficit, applied to an upland catchment in Wales. The integration has involved the use of the hybrid index-based model TOPMODEL, the HOST soil classification and the use of GIS as a spatial pre and post-processing tool.

Rather than reiterate the soil-hydrological issues discussed previously, the present chapter will attempt to place the results of the research within the wider context of ongoing and/or required research in this area.

As a preliminary consideration, we should underline that the research concentrated on an upland catchment characterised by high precipitation and shallow soils. Though such catchments may be perceived as marginal with respect to lowland catchments, they are actually very important given:

a) that they occupy about one third of the UK land surface (Neal, 1997);
b) the heightened sensitivity of both their soils and freshwater environment to acidic inputs associated with sulphate and nitrate deposition (Vincent et al., 1996);
c) the interdependence between upland afforestation – and land use changes more generally – water yields and water quality, especially given the increasing importance of upland catchments as a source of water supply (Hudson et al., 1997)

But probably most importantly of all, the research effort dedicated to the study of upland catchments such as Plynlimon has led to a conviction that "all the information now available from upland catchments must inform and guide a holistic approach to large basin management." (Hudson et al., 1997, p.396)

In developing and applying a methodology capable of such a holistic approach, a fundamental objective was to fulfill the requirements of Beven (1989, p 158). In particular, the methodology had to "explore the implications of making certain assumptions about the nature of the real world system"

and also

"predict the nature of the real world system under a set of naturally-occurring circumstances".

The critical assumptions we have made in terms of representation of physical processes were that

a) the use of the HOST-SPR index values as a surrogate for saturated hydraulic conductivity would allow us to better predict the spatially distributed soil moisture deficit;
b) the soil-topographic index used by TOPMODEL was able to represent the combined influence of soils and topography on the dynamic nature of soil water storage and release mechanisms;
c) the representation of the rainfall-runoff transformation process within the soil column, as represented by TOPMODEL, was suitable for the catchments considered.

With regard to the first assumption, the results obtained have shown how the prediction of spatially distributed soil moisture deficit was only marginally improved by incorporating the HOST-SPR index values. This result though was strongly influenced by the need to normalise the index values in order to obtain input parameters which were meaningful witin the context of TOPMODEL.

Furthermore, as Rycroft et al. (1975) already observed twenty-five years ago, well humified peat may not respect Darcian behaviour and it may therefore not be possible to define a unique saturated conductivity value as this would vary with hydraulic gradient. Consequently, an advantage of adopting the HOST SPR index approach would be to remove the need for field measured K_0 values.

Also, it would be useful to verify if the HOST SPR index is able to accurately reflect the soil water storage capacity. If so, we would be able to indirectly account for this factor even though TOPMODEL – or any other hybrid index-based model - may not explicitly consider it as an input parameter of the wetness index. Overall, the results have therefore confirmed the validity of the HOST classification, which was developed as an easily applicable dataset for the representation of soil hydrologic properties within hydrological models.

With regard to the second assumption, the simulation results have confirmed the findings of other researchers who have carried out measurements of field soil moisture and concluded that

> "no one predictive index can be expected accurately to predict surface moisture content throughout the entire drydown sequence." (Famiglietti et al., 1998, p.795)

More recent research by Western et al. (1999) has taken the above observation further and concluded that the ability of a certain index to predict soil moisture distributions depends on the degree of spatial organisation in the soil moisture values. The authors found that the spatial organisation was strongest in spring and autumn months, and weakest in the drier summer and very wet winter months. This therefore implies that for any wetness index, the ability to accurately predict soil moisture deficit may vary throughout the year and is not uniquely dependent on the soil hydrological properties.

Applying the above findings to the Plynlimon catchments, we can observe that the soil moisture patterns predicted by the present research generally exhibit a very high degree of spatial organisation. The only exceptions may be during the very high flood peaks and the longer periods of drainage, and also in the peat soils where near-saturated conditions prevail during the winter months. Though past research at Plynlimon has attempted to explain soil moisture patterns with respect to slope, soil type and aspect – which are three of the basic parameters used for defining a wetness index – the results of in-situ soil moisture measurements did not identify any significant relationships (Kirby et al., 1991). In light of the above findings, and given that the present research was only able to qualitatively validate soil moisture distributions, it would be interesting to carry out further research at Plynlimon to re-examine these issues.

Finally with regard to the third assumption, the present research has confirmed that TOPMODEL's overall representation of the runoff generating processes reflects a spatially lumped representation of soil moisture status. Essentially, the spatially distributed soil moisture deficit is controlled by the catchment average SMD which does not take fully into account the dynamic nature of saturated contributing areas. In the particular case of Plynlimon, this means that TOPMODEL is not able to model the water storage-release mechanism of the peat soils, for which the dynamics of saturation are independent from those in the hillslopes and valley bottoms. TOPMODEL instead assumes that all the saturated soil zones are permanently connected, and that therefore the flow contributing area for any point coincides with all of the upslope drained area. Beven (1997) has stated that this is probably the greatest conceptual limit of TOPMODEL and one which only the incorporation of a dynamic contributing area can overcome. This would require the calculation of a dynamic soil-topographic index, based on the true contributing areas for each cell at each timestep, and allow the catchment to function as a series of independent contributing areas.

The conclusions drawn from the present research also need to be evaluated in light of the possible application of this methodology to other catchments. In that respect we can make the following observations.

a) In terms of data requirements the approach described only requires hydrological and topographic data that is either already collected and that is generally available.
b) Within the context of UK upland catchments (with extensive peat soils coverage) the methodology described is likely to lead to similar results in terms of outflow. What remains to be validated are the actual soil moisture deficit predictions, which would require an intensive field measurement study.

c) Within the more general context of lowland catchments, where there is likely to be less variability in topography and a more homogeneous distribution of soils, the effect of a spatially variable K_0 on soil moisture deficit may be more significant.

d) With regards to the development of a dynamic soil-topographic index, it will be necessary to evaluate the impact of reduced contributing areas on the calibrated K_0avg value(s). It may well be that to compensate for the more realistic values of contributing area, the calibrated K_0avg will also decrease. This in turn may lead to more physically realistic K_0avg values, and therefore to the possibility that actual published values may be used instead of a normalised K_0 like the HOST-SPR index.

In their application of TOPMODEL for the prediction of water table depths in shallow forest soils, Moore and Thompson (1996, pg 669) called for further research to

> "specify more clearly the bounds of applicability of the underlying (TOPMODEL) assumptions and to identify workable extensions and modifications to the concept, where necessary."

The present research has concentrated on evaluating such boundaries, and has hopefully contributed to a greater understanding of the specific limitations of all hybrid index-based modes with regards to the prediction of spatially distributed soil moisture deficit.

Looking ahead towards a more widespread applicability of integrated hydrological models, spatially variable soil data and GIS, the present research has considered some of the key issues which are crucial to future successful applications. In particular, building on the ideas of Moore et al. (1993) and Grayson et al. (1993), the present research has:

a) evaluated the feasibility of using easily accessible soil hydrological properties data, in this specific case using the HOST classification;

b) attempted a qualitative interpretation of physical patterns (eg. soil moisture deficit) as a function of soil hydrologic properties and physical process understanding;
c) confirmed the benefits of integration with GIS, especially with regards to a more qualitative approach to the validation of spatially distributed soil moisture deficit;
d) confirmed the need for detailed field studies that explore spatio-temporal variability of soil moisture distribution, both to support model validation and also to evaluate the suitability of wetness indices;

The consideration of the above issues in the present research has allowed a qualitative evaluation of SMD predictions with respect to soil hydrological properties and, hopefully, yielded a new perspective on the dynamics of soil moisture deficit within the Plynlimon catchments.

More broadly though, the present research has evaluated a methodology capable of both integrating diverse process modelling and spatial data handling approaches, while providing a critical analysis tool for better understanding catchment behaviour. It is hoped that the results presented will be seen as a valid contribution to the debate on hydrology's future, as summarised by Entekahbi et al. (1999), and thus help to answer some of the crucial hydrological issues facing society.

Bibliography

List of Abbreviations

Bull. Am. Met. Soc.	*Bulletin of the American Meteorological Society*
Bull. Int. Ass. Hydrol. Sci.	*Bulletin of the International Association of Hydrological Sciences*
C.R.E.S.	*Centre for Research in Environmental Sciences*
Hydr. Sci. J.	*Hydrological Sciences Journal*
Hydr. Processes	*Hydrological Processes*
Hydr. Sci. Bull.	*Hydrological Sciences Bulletin*
I.A.H.S.	*International Association of Hydrological Sciences*
Int. J. of GIS	*International Journal of Geographic Information Systems*
J. Geology	*Journal of Geology*
J. Hydrol.	*Journal of Hydrology*
J. Institution of Soil and Water Management	*Journal of the Institution of Soil and Water Management*
N.E.R.C.	*Natural Environment Research Council*
Soil Sci. Soc. Am. J.	*Soil Science Society of America Journal*
S.S.L.R.C.	*Soil Survey Land Research Centre*
Water Resour. Res.	*Water Resources Research*

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Appendices

Appendix 1

The present appendix lists the Fortran source code developed and used in the present research project.

a) The data conversion utilities (grid_exp.for & grid_imp.for) used to export and import files from ARC to the ASCII format required by TOPMODEL.
b) The modified TOPMODEL source code with the changes carried out to incorporate a spatially variable saturated soil conductivity.
c) The soil moisture deficit program (smderr.for) used to calculate the SMD maps and the SMD difference maps.

A) Data Conversion Utilities

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
      Program grid_exp
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c     This program reformats GRID files exported by ARC/INFO,
c     from row-major order to x,y,z columns. Program also changes
c     all NODATA values to -9999.0, counts total no. of data
c     values in file, as well as total no. of valid grid cells.
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c

      implicit none
c
      integer cells,count,nrow,ncol,size,null,x,y,ierr
      real area,col(76),dtm(500,500),xll,yll,sum,avg
      character*60 infile,outfile,formfile
      logical last
c
      print*,' Name of input file?'
      read(*,10) infile
      print*,' Name of formatted file?'
      read(*,10) formfile
      print*,' Name of output file?'
      read(*,10) outfile
   10 format(A12)
      print*
c
      open(unit=30,file=infile,status='old',form='formatted')
      open(unit=31,file=formfile,status='unknown',form='formatted')
      open(unit=33,file=outfile,status='unknown',form='formatted')
c
      read(30,20)ncol
      read(30,20)nrow
      read(30,25)xll
      read(30,25)yll
      read(30,20)size
      read(30,20)null
      write(31,30)ncol,nrow,xll,yll,size,null
c
   20 format(14x,i5)
   25 format(14x,f10.0)
   30 format(1x,'No. of columns = ',i5,/
     &       1x,'No. of rows    = ',i5,/
     &       1x,'DEM (xll,yll)  = ',2f10.0,/
     &       1x,'Cell Size      = ',i5,/
     &       1x,'NODATA Value   = ',i5,//,
     &       1x,'N.B. Though the DEM (xll,yll) coordinates are
     &       1x,'given,the actual row numbering',/
     &       1x,'starts from the top left corner of the DEM.',/)
c
c     READ IN DATA FROM FILE
c
      do 40 y = 1,nrow
         read(30,*,iostat=ierr,err=40)(dtm(x,y),x=1,ncol)
   40 continue
c
      do 80 y=1,nrow
         write(31,50)y
         write(31,60)(dtm(x,y),x=1,ncol)
```

```
   50     format(I5)
   60     format(9(8F10.2,/),4F10.2,/)
   80  continue
c
       last=.false.
       sum=0.0
       count=0
       cells=0
       do 180 y=1,nrow
         do 170 x=1,ncol
         if(.not.last)then
           if(dtm(x,y).gt.-99999.0)then
             count=count+1
             if(dtm(x,y).le.0.0) then
               dtm(x,y)=-9999.9
             else
               cells=cells+1
               sum=sum+dtm(x,y)
             endif
             write(33,160)x,y,dtm(x,y)
 160         format(1x,2i4,f11.4)
           else
             last=.true.
           endif
         endif
 170    continue
 180   continue
 190   continue
       PRINT *, 'TOT. NO OF VALUES READ IN  = ',COUNT
       PRINT *, 'TOT. NO OF VALID DEM CELLS = ',CELLS
c
       AREA=SIZE*SIZE*CELLS
       PRINT *, 'CATCHMENT AREA (m2)        = ',AREA
c
       avg=sum/cells
       PRINT *, 'SPATIALLY AVERAGED VALUE   = ',AVG
c
       close(30)
       close(31)
       close(33)
       end
```

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
C
      Program grid_imp
C
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
C
C     This program reformats DTM file created by TOPMODEL into
C     formats required by ARC-INFO [ASCIIGRID in GRID]. It
C     assumes that origin of input DTM is in upper left corner,
C     as in GRID.
C
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
C

      implicit none
c
      integer x,y,ierr,i,j,
     &        ncol,nrow,xll,yll,size,null
      real dtm(500,500)
      character*60 infile,outfile,datafile
c
      print*,' Name of input file?'
      read(*,10) infile
      print*,' Name of GRID data file?'
      read(*,10) datafile
      print*,' Name of output file?'
      read(*,10) outfile
   10 format(A12)
      print*
c
      open(unit=30,file=infile,status='old',form='formatted')
      open(unit=31,file=datafile,status='old',form='formatted')
      open(unit=33,file=outfile,status='unknown',form='formatted')
c
      read(31,20)ncol
      read(31,20)nrow
      read(31,25)xll
      read(31,25)yll
      read(31,20)size
c     read(31,20)null
      null=0
      write(33,30)ncol,nrow,xll,yll,size,null
c
   20 format(14x,i5)
   25 format(14x,i10)
   30 format('ncols          ',i3/
     &       'nrows          ',i3/
     &       'xllcorner      ',i6,/
     &       'yllcorner      ',i6,/
     &       'cellsize       ',i2,/
     &       'NODATA_value   ',i1)
c
      print*,' Reading in data...'
c
      do 50 j=1,nrow
        do 40 i=1,ncol
         dtm(i,j)=0.0
   40   continue
   50 continue
c
```

```
      do 100 j=1,nrow
        do 90 i=1,ncol
          read(30,*,iostat=ierr,err=50) x,y,dtm(i,j)
          if(dtm(i,j).le.-9999.0) dtm(i,j)=0.0
   90   continue
  100 continue
c
c     Write data to format required by ASCIIGRID ....
c
      print*,' Writing out data...'
c
      do 150 j=1,nrow
         write(33,130)(dtm(i,j),i=1,ncol)
  130    format(76(F9.4))
  150 continue
c
      close(30)
      close(31)
      close(33)
      end
```

B) TOPMODEL Programs

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      COMMON.FOR
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBPROGRAM DECLARES ALL THE VARIABLES TO BE USED IN
C      THE PROGRAM TOPMODEL. NO VARIABLE HAS A DEFAULT TYPE AND
C      ALL ARE DECLARED. THEREFORE IMPLICIT NONE IS USED TO CHECK
C      THAT THIS IS STRICTLY ADHERED TO.
C
C      THE DATA SPACE ALLOCATION ALLOWS 1 YEARS WORTH OF ANALYSES
C      AT THE MOMENT AND CAN BE CHANGED BY ALTERING "TIME" IN THE
C      PARAMETER LIST. THE MAX. NUMBER OF LN (A/TAN B) INCREMENTS
C      IT WILL ALLOW IS 40 INCREMENTS, WHICH CAN BE ALTERED BY
C      EDITING THE "NUMINC" PARAMETER. THE NUMBER OF BANDS ALLOWED
C      FOR IS 15 IN THE "NUMBAN" PAPRAMETER AND THE NUMBER OF
C      HEADWATER SUBCATCHMENT ALLOWED FOR IS 5 IN THE "NUMHED"
C      PARAM
C
C      N.B. FOR THE SIMULATIONS CARRIED OUT NUMBAN AND NUMHED ARE
C      ALWAYS ASSUMED EQUAL TO ONE.
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
       IMPLICIT NONE
       INTEGER TIME,NUMINC,NUMBAN,NUMHED,XDIM,YDIM
       PARAMETER (TIME =9000,
     &            NUMINC=40,
     &            NUMBAN=15,
     &            NUMHED=5,
     &            XDIM=500,
     &            YDIM=500)
C
C      GIVING EACH VARIABLE A SPECIFIC VARIABLE TYPE
C
       INTEGER NUMACT,NHEAD,NBAND,NGAUGE,MAX,HEAD,BAND,ATB,DELAY,NT,
     &         IT,I,J,ITER,NCALL,NOWT,NY,NX,TSTART,TEND,K0STATUS,X,Y,
     &         CORR,FULL,EFFITER,RUN
C
       REAL M,SK0,SRMAX,ALPHA,CHV,QINITL,T0,MINATB,MAXATB,STEPA,
     &      ATOB,A,SUMATB,NOBAND,GAMMA,Q0,NOHEAD,TOTALA,NUMATB,DIST,
     &      SBAR,QOBS,R,E,ROFF,EX,EX1,EX2,P,S,SRZ,SUZ,EA,QUZ,QB,QV,
     &      QBAND,QHEAD,QALL,Q,SUMOBS,SUMSIM,SUMR,SUME,NATB,ATBVAL,
     &      ACQB,ACQV,ACSE,ACSU,ACAE,SUBQB,SUBQV,SUBSE,SUBSU,SUBAE,
     &      BALINI,BALEND,ALLATB,ALLGAM,ALLQ0,ALSBAR,ENSBAR,BUDGET,
     &      QOBAR,SSE,VARI,EFF,GAUGE,
     &      ATOBVAL,LNATANB,DIFFSQ,SUBATOB,TOTQ1,TOTQ2,TOTQ3,
     &      TROFF1,TROFF2,TQV,
     &      SUBAREA,QSUB,SUMSUB
C
C      The following variables have been defined for the case of a
C      spatially variable K0.
C
       REAL ATANB,AVGK0,MEANATOB,MEANK0,MEANT0,SUMK0,SUMT0,SUMATOB
C
       CHARACTER*10 NAME
       CHARACTER*15 SOILFILE
C
```

```
      COMMON /CPREAD/QOBS(TIME,NUMHED),R(TIME,NUMHED),
     &               E(TIME,NUMHED),IT,NOWT
C
      COMMON /CTREAD/EFFITER,M,SK0,SRMAX,ALPHA,CHV,QINITL,T0,I,J,
     &               NUMACT,NHEAD,NBAND,MINATB,MAXATB,STEPA,MAX,
     &               NGAUGE,GAUGE(NUMHED),NUMATB,TSTART,TEND,NT,
     &               K0STATUS,CORR,NY,NX,
     &               DIST(NUMBAN),HEAD,BAND,ATB,A(NUMINC),ATBVAL,
     &               ATOB(XDIM,YDIM),NATB(NUMHED,NUMBAN,NUMINC),
     &               SUMATB(NUMHED,NUMINC),NOBAND(NUMHED,NUMBAN),
     &               NOHEAD(NUMHED),GAMMA(NUMHED,NUMBAN),
     &               SBAR(NUMHED,NUMBAN),Q0(NUMHED,NUMBAN),TOTALA,
     &               BALINI,ALLATB,ALLGAM,ALLQ0,ALSBAR,
     &               ACQB,ACQV,ACSU,ACSE,ACAE,
     &               SUBQB(NUMHED),SUBQV(NUMHED),SUBSE(NUMHED),
     &               SUBSU(NUMHED),SUBAE(NUMHED),
     &               ATANB(XDIM,YDIM),AVGK0(NUMHED),
     &               MEANATOB(NUMHED),MEANK0(NUMHED),
     &               MEANT0(NUMHED),SUMK0,SUMT0,SUMATOB
C
      COMMON /CTOPMOD/ITER,ROFF,QV,EX,EX1,EX2,P,EA,QUZ,QB,FULL,
     &               S(NUMHED,NUMBAN,NUMINC),
     &               SRZ(NUMHED,NUMBAN,NUMINC),
     &               SUZ(NUMHED,NUMBAN,NUMINC),
     &               NAME
C
      COMMON /CROUTE/DELAY,QHEAD,QBAND,Q(TIME,NUMHED),QALL,
     &               QSUB(TIME),SUBAREA
C
      COMMON /CRESULTS/SUMSIM(NUMHED),SUMOBS(NUMHED),
     &                 SUMR(NUMHED),SUME(NUMHED),SUMSUB,
     &                 SOILFILE
C
      COMMON /CWATBAL/RUN,QOBAR(NUMHED),SSE(NUMHED),VARI(NUMHED),
     &                ENSBAR,BALEND,EFF(NUMHED),BUDGET(NUMHED)
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     MODIFIED TOPMODEL CODE, WRITTEN BY MAURO CIACCIO
C     UNIVERSITY OF EDINBURGH, DEPT. OF GEOGRAPHY, 1999
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      PROGRAM MAIN
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     LOAD ALL INPUT DATA FILES FROM "RUN" FILE
C
      INTEGER NRUNS,COUNT
      CHARACTER*15 RUNFILE,INPUTS1$,INPUTS2$,SUBCAT$,PARAMS$,
     &             OUTPUT1$,OUTPUT2$,EXCEL$
      CHARACTER*80 TITLE
C
      OPEN(1000,FILE="PLYN.RUN",STATUS="OLD")
C
      READ(1000,"(A)")TITLE
      READ(1000,"(A)")PARAMS$
      READ(1000,"(A)")SUBCAT$
      READ(1000,"(A)")INPUTS1$
      READ(1000,"(A)")INPUTS2$
C     SPATIALLY VARIABLE K0 FLAG
      READ(1000,*) K0STATUS
      READ(1000,"(A)") SOILFILE
      if(k0status.eq.1) then
        print *,'Soil classification file: ',SOILFILE
        print *
      endif
C     CORRECTION TO MEAN K0 FLAG
      READ(1000,*) CORR
C     CALCULATION OF SUBCATCHMENT SUBTOTALS FLAG
      READ(1000,*) FULL
C     PARAMETER ITERATION FLAG
      READ(1000,*) EFFITER
      READ(1000,*)
      READ(1000,"(A)")EXCEL$
      READ(1000,"(A)")OUTPUT1$
      READ(1000,"(A)")OUTPUT2$
C
    5 OPEN(1,FILE=SOILFILE,STATUS="OLD")
      OPEN(5,FILE=PARAMS$,STATUS="OLD")
      OPEN(10,FILE=SUBCAT$,STATUS="OLD")
      OPEN(15,FILE=INPUTS1$,STATUS="OLD")
      OPEN(16,FILE=INPUTS2$,STATUS="OLD")
      OPEN(21,FILE=OUTPUT1$,STATUS="UNKNOWN")
      OPEN(22,FILE=OUTPUT2$,STATUS="UNKNOWN")
      OPEN(30,FILE=EXCEL$,STATUS="UNKNOWN")
C
      WRITE(21,1001)TITLE
      WRITE(22,1001)TITLE
 1001 FORMAT(1x,A,)
C
C***************************************************************
```

```
C     CALLING SUBROUTINES
C
C     INITIALISING ALL ARRAYS AND VARIABLES
      CALL INIMOD
C
C     READING IN CATCHMENT PARAMETERS, CATCHMENT STRUCTURE AND
C     TOPOGRAPHIC INFORMATION
      CALL TREAD
C
C     READING IN HYDROLOGICAL DATA, RAINFALL, EVAPORATION AND
C     OBSERVED FLOWS
      CALL PREAD
C
C     RUNNING TOPMODEL
      CALL TOPMOD
C
C     PRINTING OUT THE RESULTS
      CALL RESULTS
C
C     GENERATING SUMMARY INFZRMATION ABOUT THE MODEL
      CALL WATBAL
C
      END
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE INIMOD
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      DO 10 HEAD=1,NUMHED
        NOHEAD(HEAD)=0.0
        GAUGE(HEAD)=0.0
        SUMSIM(HEAD)=0.0
        SUMOBS(HEAD)=0.0
        SUMR(HEAD)=0.0
        SUME(HEAD)=0.0
        SUBQB(HEAD)=0.0
        SUBQV(HEAD)=0.0
        SUBSE(HEAD)=0.0
        SUBSU(HEAD)=0.0
        SUBAE(HEAD)=0.0
        DO 20 BAND=1,NUMBAN
          NOBAND(HEAD,BAND)=0.0
          SUMATB(HEAD,BAND)=0.0
          GAMMA(HEAD,BAND)=0.0
          Q0(HEAD,BAND)=0.0
          SBAR(HEAD,BAND)=0.0
          DO 30 ATB=1,NUMINC
            A(ATB)=0.0
            NATB(HEAD,BAND,ATB)=0
            S(HEAD,BAND,ATB)=0.0
            SUZ(HEAD,BAND,ATB)=0.0
C
C           SRZ IS INITIALISED AFTER SRMAX IS READ IN
C
   30     CONTINUE
   20   CONTINUE
   10 CONTINUE
      TOTALA=0.0
      QBAND=0.0
      QHEAD=0.0
      QALL=0.0
```

```
      MAX=0
      P=0.0
      ROFF=0.0
      TROFF1=0.0
      TROFF2=0.0
      TQV=0.0
      EA=0.0
      ACQB=0.0
      ACQV=0.0
      ACSE=0.0
      ACSU=0.0
      ACAE=0.0
      QOBAR=0.0
      SSE=0.0
      VARI=0.0
      BALINI=0.0
      ALLATB=0.0
      ALLGAM=0.0
      ALLQ0=0.0
      ALSBAR=0.0
      BALEND=0.0
      ENSBAR=0.0
      EFF=0.0
      DO 40 HEAD=1,NUMHED
        DO 50 IT=1,TIME
          QOBS(IT,HEAD)=0.0
          R(IT,HEAD)=0.0
          E(IT,HEAD)=0.0
          Q(IT,HEAD)=0.0
   50   CONTINUE
   40 CONTINUE
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE TREAD
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C !!! SUBROUTINE HAS BEEN MODIFIED TO ALLOW SPATIALLY VARIABLE SKO
C
C     DEFINING VAR. TYPES EXCLUSIVELY FOR THIS SUBROUTINE
C
      INTEGER DUM1,DUM2,CELLS,ERRCOUNT,TOT,MAXSTAT,MAXCLASS(NUMHED)
C
      REAL A1,A2,ATNB,ATOBINI,ATOBEND,
     &     ATOBDIST(NUMHED,NUMBAN,NUMINC),ATOBMIN,K0(XDIM,YDIM),
     &     K0CORR(NUMHED),MAXATOB,MINATOB,T00(XDIM,YDIM)
C
      OPEN(120,FILE='ATOB_DIS.DAT',STATUS='UNKNOWN')
      OPEN(125,FILE='a_input.DAT',STATUS='UNKNOWN')
C     OPEN(200,FILE='ZSUMINFO.DAT',STATUS='unknown')
C
C     READING IN THE CONTROL PARAMETERS
C
      READ(5,*)
      IF(EFFITER.EQ.1)THEN
        READ(5,*) M,SRMAX,SK0,ALPHA,CHV
      ELSE
        READ(5,*) M,SRMAX,SK0,ALPHA,CHV
      ENDIF
```

```
C
C     READ IN THE MODEL STRUCTURE CONTROLS
C     ("NUMACT" comes from original version of code, and it
C      defines the max. number of subcatchments, each of which can
C      have a max. of NHEAD headwaters and NBAND distance bands.
C      NOT USED in my simulations, because I effectively define
C      subcatchments only with 1 headwater!)
C
      READ(5,*) NUMACT,NHEAD,NBAND,MINATB,MAXATB,STEPA
C
C     READING IN THE STARTING POSITION AND THE NUMBER
C     OF TIMESTEPS THAT THE SIMULATION WILL RUN
C
      READ(5,*)
      READ(5,*) TSTART,TEND,QINITL
C
      NT=(TEND-TSTART)+1
      print *,'Number of timesteps = ',NT
      print *,'Running...'
C
C     READ IN THE GAUGE DATA AS DISTANCES FROM THE OUTFALL
C     THE OUTFALL GAUGE IS GIVEN A DEFAULT DISTANCE OF 0.0
C
      READ(5,*) NGAUGE
      print *,'No. of flow gauges = ',ngauge
      DO 30 I=1,NGAUGE
        READ(5,*) GAUGE(I)
        print *,'Distance of gauge ',I,' = ',gauge(I)
   30 CONTINUE
C
C     READING IN THE DISTANCE TO THE START OF EACH BAND
C
      DO 40 I=1,NBAND
        READ(5,*) DIST(I)
        print *,'Distance of band ',I,' = ',dist(I)
   40 CONTINUE
C
      CLOSE(5)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     CALCULATION OF a/T0*tanB DISTRIBUTION
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      PRINT *
      PRINT *,'Is saturated conductivity (K0) spatially variable?'
      PRINT *,'If YES type "1"; if NO type "2":',K0STATUS
      PRINT *
C
C     BEGIN LOOP THAT CALCULATES a/T0tanb DISTRIBUTION.
C
C     IF K0 is constant
C          - calculate or assign T0 and MAX
C          - read in a/tanb distribution, which will be the
C            same as the a/T0tanb distribution
C          - calculate values of a/T0tanb
C          - write out results to 'a_input.dat'
C
      OPEN(100,FILE='GRID.DAT',STATUS='OLD')
      READ(100,*) NX,NY
C
      IF (K0STATUS.EQ.2) THEN
         T0=SK0*M
```

```
C
C       PRINT *
C       PRINT *, 'Specify no. of ln(a/T0tanb) classes?'
C       PRINT *, 'If YES type "1"; if NO type "2".'
C       READ (*,*) MAXSTAT
C       PRINT *
        MAXSTAT=2
        IF(maxstat.eq.1)THEN
          PRINT *, 'Assign value of MAX:'
          READ (*,*) MAX
          stepa=((maxatb-minatb)/max)
        ELSE
          MAX=INT((MAXATB-MINATB)/STEPA)
          WRITE(125,45)MAX
        ENDIF
   45   FORMAT(1X,'No. of a/T0*tanb classes = ',I3,/)
C
C       Necessary to insert a loop to read subcatchment
C       ln(a/tanB) distributions.....
C
        DO 55 I=1,NHEAD
          DO 50 ATB=1,MAX
            READ(10,*) DUM1,HEAD,BAND,ATNB,NUMATB
            NATB(HEAD,BAND,ATB)=NATB(HEAD,BAND,ATB)+NUMATB
   50     CONTINUE
   55   CONTINUE
C
C       Calculating (a/Totanb) for each a/tanb class...
C       Writing out results to 'ATOBDIS.DAT'...
C
        ATNB=MINATB
        WRITE(120,60)
   60   FORMAT(1X,'ATB    LNATNB    LNAT0B   NATB',/)
        DO 75 HEAD=1,NHEAD
          DO 70 ATB=1,MAX
           A(ATB)=ATNB-ALOG(T0)
           IF(A(ATB).LE.0.0) A(ATB)=0.0
           WRITE(120,65) ATB,ATNB,A(ATB),NATB(HEAD,BAND,ATB)
           ATNB=ATNB+STEPA
   65      FORMAT(1X,I3,3F10.3)
   70     CONTINUE
          ATNB=MINATB
   75   CONTINUE
C
        CLOSE(10)
C
     ELSE
C          - read in DEM size, ATANB(x,y) and K0(x,y) arrays
C          - calculate ATOB(X,Y), MAXATOB and MINATOB and write out
C            results to file 'ATob.dat'
C          - calculate a/T0tanb distribution, with procedure
C            analogous to that used in MATB.FOR to calculate a/tanb
C            distribution.
C          - write out A(ATB) and NATB(HEAD,BAND,ATB) to 'ATOB.DAT'
C
        OPEN(115,FILE='ATOB.DAT',STATUS='UNKNOWN')
C
C       BEGIN SUBCATCHMENT LOOP...
C
        BAND=0
        DO 180 HEAD=1,NHEAD
         BAND=BAND+1
C
          OPEN(105,FILE='YFREEATB.DAT',STATUS='OLD')
```

```
      PRINT*,'**********************************************'
      PRINT*,'ARE YOU USING THE CORRECT YFREEATB.DAT FILE???'
      PRINT*,'**********************************************'
      PRINT*
C
      READ(1,80) DUM1, AVGK0(HEAD)
 80   FORMAT(1X,I3,F6.4)
C
      PRINT*,'Subcatchment / distance band    =',head,'/',band
      PRINT*
      PRINT *, 'Correct K0 values by SK0/(Avg. K0)?'
      PRINT *, 'If YES type "1"; if NO type "2":',CORR
      PRINT *
      IF(CORR.EQ.1)THEN
        K0CORR(HEAD)=SK0/AVGK0(HEAD)
      ELSE
        K0CORR(HEAD)=1
      ENDIF
      PRINT *,'K0CORR = ',K0CORR(HEAD)
      PRINT *
C     WRITE(115,*) 'K0CORR = ',K0CORR(HEAD)

      CELLS=0

      SUMK0=0
      SUMT0=0
      SUMATOB=0
      ERRCOUNT=0
      MAXATOB=0.00
      MINATOB=100.00
      MAX=0
      TOT=0
      WRITE(115,81)
 81   FORMAT(1X,'  X  Y   A/TOTANB')
C
C     BEGIN X,Y LOOPS
C
      READ(105,*)
      DO 100 Y=1,NY
       DO 90 X=1,NX
C
         READ(105,*) I,J,ATANB(X,Y)
         READ((HEAD),*) DUM1,DUM2,K0(X,Y)
         IF(K0(X,Y).GT.0.0)THEN
            K0(X,Y)=K0CORR(HEAD)*K0(X,Y)
         ELSE
            ERRCOUNT=ERRCOUNT+1
         ENDIF
C
         T00(X,Y)=M*K0(X,Y)
C
         IF((ATANB(X,Y).LT.2990.0).AND.(K0(X,Y).GT.0.0))THEN
            ATOB(X,Y)=ATANB(X,Y)-(ALOG(T00(X,Y)))
         ELSE
            ATOB(X,Y)= 2999.0
         ENDIF
C
C        WRITING ATOB(X,Y) VALUES TO FILE ATOB.DAT
C
         WRITE(115,85)I,J,ATOB(X,Y)
 85      FORMAT(1X,2I3,F12.6)
C
         IF (ATOB(X,Y).LT.100) THEN
            IF(MAXATOB.LT.ATOB(X,Y)) THEN
```

```
                    MAXATOB=ATOB(X,Y)
                 ELSE IF(MINATOB.GT.ATOB(X,Y)) THEN
                    MINATOB=ATOB(X,Y)
                 ENDIF
              ELSEIF((ATOB(X,Y).LT.2999.0).AND.
     &                   (ATOB(X,Y).GE.100.0)) THEN
                 PRINT *,' LNATOB>100 FOR X,Y = ',X,Y
              ENDIF
              IF((ATOB(X,Y).LT.100.0).AND.(ATOB(X,Y).GT.0.0)) THEN
                SUMK0=SUMK0+K0(X,Y)
                SUMT0=SUMT0+T00(X,Y)
                SUMATOB=SUMATOB+ATOB(X,Y)
                CELLS=CELLS+1
              ENDIF
C
  90        CONTINUE
 100       CONTINUE
C
C          Verifying no of valid cells in subcatchment
           IF(ERRCOUNT.EQ.NX*NY) THEN
             PRINT*,'NO VALID CELLS IN SUBCATCHMENT'
             PRINT*
           ELSE
             MEANK0(HEAD)=(SUMK0/CELLS)
             MEANT0(HEAD)=(SUMT0/CELLS)
             MEANATOB(HEAD)=(SUMATOB/CELLS)
             PRINT*,'Number of valid DEM cells    =',cells
             PRINT*,'Sum of K0 values             =',sumk0
             PRINT*,'Spatially averaged K0        =',meank0(HEAD)
             PRINT*,'Sum of T0 values             =',sumt0
             PRINT*,'Spatially averaged T0        =',meant0(HEAD)
             PRINT*,'Sum of ln(a/T0tanb) values   =',sumatob
             PRINT*,'Spatially avg. ln(a/T0tanb)  =',meanatob(HEAD)
             PRINT*
           ENDIF
C
C          IF K0CORR=1, THEN SK0 SHOULD BE SET TO MEANKO(1)
C
           IF(K0CORR(HEAD).EQ.1)THEN
             SK0=MEANK0(1)
           ENDIF
C
           MAXCLASS(HEAD)=INT((MAXATOB-MINATOB)/STEPA)
           IF(MAXCLASS(HEAD).GT.MAX) MAX=MAXCLASS(HEAD)
           IF(MINATOB.GE.0.0)THEN
              ATOBINI=INT(MINATOB)
           ELSE
              ATOBINI=0.0
           ENDIF
           ATOBEND=ATOBINI+(MAX*STEPA)
           WRITE(125,105)HEAD,BAND,MINATOB,MAXATOB,ATOBINI,ATOBEND,
     &                    MAX
 105       FORMAT(/,1X,'Subcatchment & distance band    =',2I3,/
     &              1X,'Min value of a/To*tanb   = ',F7.2,/
     &              1X,'Max value of a/To*tanb   = ',F7.2,/
     &              1X,'Lowest a/To*tanb class   = ',F7.2,/
     &              1X,'Highest a/To*tanb class  = ',F7.2,/
     &              1X,'No. of a/To*tanb classes = ',I7,/)
           DO 110 ATB=1,MAX
             ATOBDIST(HEAD,BAND,ATB)=0.0
 110       CONTINUE
C
C          Calculating no. of cells in each a/Totanb class...
C
```

```
            ATOBMIN=ATOBINI
            DO 130 Y=1,NY
             DO 125 X=1,NX
               IF (ATOB(X,Y).GE.2990.0) THEN
                 ATB=0
               ELSE IF (ATOB(X,Y).LE.ATOBINI) THEN
                 ATOBDIST(HEAD,BAND,1)=ATOBDIST(HEAD,BAND,1)+1
C                ATB=1
               ELSE IF (ATOB(X,Y).GT.ATOBEND.AND.
     &                 ATOB(X,Y).LT.100.0) THEN
                 ATOBDIST(HEAD,BAND,MAX)=ATOBDIST(HEAD,BAND,MAX)+1
               ELSE
                 DO 115 ATB=1,MAX
                  A1=ATOBMIN
                  A2=ATOBMIN+STEPA
                  IF ((ATOB(X,Y).GT.A1).AND.(ATOB(X,Y).LE.A2)) THEN
                    ATOBDIST(HEAD,BAND,ATB)=ATOBDIST(HEAD,BAND,ATB)+1
                  ENDIF
                  ATOBMIN=ATOBMIN + STEPA
  115            CONTINUE
               ENDIF
               ATOBMIN=ATOBINI
  125        CONTINUE
  130       CONTINUE
C
C           Writing out no. of cells in each class to
C           'atobdist.dat'...
C
            ATOBMIN=ATOBINI
            WRITE(120,135)
  135       FORMAT(1X,'ATB  LNATOB    NATB       TOT',/)
            DO 145 ATB=1,MAX
              TOT=TOT+ATOBDIST(HEAD,BAND,ATB)
              NATB(HEAD,BAND,ATB)=ATOBDIST(HEAD,BAND,ATB)
              A(ATB)=ATOBMIN
              WRITE(120,140)ATB,A(ATB),NATB(HEAD,BAND,ATB),TOT
              ATOBMIN=ATOBMIN + STEPA
  140         FORMAT(1X,I3,F7.3,F10.3,I7)
  145       CONTINUE
C
C           Writing out results to 'a_input.dat'...
C
            WRITE(125,150)
  150       FORMAT(1X,'HEAD BAND  ATB    LNATOB    NATB',/)
            DO 160 ATB=1,MAX
              WRITE(125,155) HEAD,BAND,ATB,A(ATB),NATB(HEAD,BAND,ATB)
  155         FORMAT(1X,3I5,2F10.3)
  160       CONTINUE
C
           CLOSE (105)

C          ENDING SUBCATCHMENT LOOP
C
  180     CONTINUE
C
C         Close soil files...
          DO 600 I=1,NGAUGE
            CLOSE(I)
  600     CONTINUE
C
C         Set max. class size
          IF(MAXCLASS(1).GE.MAXCLASS(2)) THEN
           MAX=MAXCLASS(1)
          ELSE
```

```
          MAX=MAXCLASS(2)
         ENDIF
C        PRINT*,MAX,MAXCLASS(1),MAXCLASS(2)
C
      ENDIF
C
      CLOSE (100)
C
C     END OF MODIFICATIONS FOR CALCULATION OF LN(A/TO*TANB)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      WRITE(125,185)
  185 FORMAT(1X,'head band atb a(atb)    natb    sumatb
     noband',/)
C
      DO 220 HEAD=1,NHEAD
C       PRINT*,'HEAD =',HEAD
        DO 210 BAND=1,NBAND
C         PRINT*,'BAND =',BAND
          DO 200 ATB=1,MAX
C           PRINT*,'ATB =',ATB
C
C      INITIALISING THE VALUE OF ALL THE SRZ STORES
C
            SRZ(HEAD,BAND,ATB)=SRMAX
C
C      SUMMING THE TOTAL NUMBER OF CELLS WITHIN EACH ATB INCREMENT
C      AND CALCULATING THERE CORRESPONDING PROPORTIONS SO AS TO
C      DETERMINE GAMMA
C
            SUMATB(HEAD,BAND)=SUMATB(HEAD,BAND)+
     &                        NATB(HEAD,BAND,ATB)*A(ATB)
            NOBAND(HEAD,BAND)=NOBAND(HEAD,BAND)+NATB(HEAD,BAND,ATB)
            WRITE(125,190)HEAD,BAND,ATB,A(ATB),NATB(HEAD,BAND,ATB),
     &                    SUMATB(HEAD,BAND),NOBAND(HEAD,BAND)
  190       FORMAT(1X,3I3,4F10.3)
C
  200     CONTINUE
C
C     IF THERE IS NO AREA WITHIN THE CLASS THEN SKIP OUT OF THE
C     CALCULATIONS TO AVOID FLOATING DIVIDE BY ZERO ERRORS
C
          IF(NOBAND(HEAD,BAND).GT.0.0) THEN
            ALLATB=ALLATB+SUMATB(HEAD,BAND)
            GAMMA(HEAD,BAND)=SUMATB(HEAD,BAND)/NOBAND(HEAD,BAND)
            Q0(HEAD,BAND)=EXP(-GAMMA(HEAD,BAND))
            NOHEAD(HEAD)=NOHEAD(HEAD)+NOBAND(HEAD,BAND)
C
            PRINT *,'The value of SUMATB is: ', SUMATB(HEAD,BAND)
            PRINT *,'The value of NOBAND is: ', NOBAND(HEAD,BAND)
            PRINT *,'The value of gamma is:  ', gamma(HEAD,BAND)
            PRINT *,'The value of Q0 is:     ', Q0(HEAD,BAND)
C           PRINT*
C
          ELSE
            WRITE(125,*) ' NO CELLS IN SUBCATCHMENT!!!'
          ENDIF
C
  210   CONTINUE
C
        TOTALA=TOTALA+NOHEAD(HEAD)
C
  220 CONTINUE
```

```
C
C     HERE THE WATER BALANCE INFORMATION FOR HOW MUCH WATER IS IN
C     THE STORES IS CALCULATED. SUZ IS EMPTY AND SRZ=SRMAX SO THE
C     WATBAL IN UNITS FOR THE WHOLE CATCHMENT IS SRMAX
C     A CATCHMENT AVERAGE SBAR VALUE IS CALCULATED FOR THE
C     WATER BALANCE CALCULATIONS IN WATBAL
C
      BALINI=SRMAX
      ALLGAM=ALLATB/TOTALA
      ALLQ0=EXP(-ALLGAM)
      ALSBAR=-M*(ALOG(QINITL/ALLQ0))
C
      WRITE(125,230) ALLATB,BALINI,ALLGAM,ALLQ0,ALSBAR
  230 FORMAT(1X,'ALLATB                 = ',F10.3/
     &       1X,'BALINI=SRMAX           = ',F10.3/
     &       1X,'ALLGAM=ALLATB/TOTALA = ',F10.3/
     &       1X,'ALLQ0=EXP(-ALLGAM)     = ',F10.3/
     &       1X,'ALSBAR=-M*(ALOG(QINITL/ALLQ0))  = ',F10.3/)
C
      IT=0
      DO 250 HEAD=1,NHEAD
        DO 240 BAND=1,NBAND
C
C     QIN WILL BE CALCULATED IN UNITS FOR THE TOTAL CATCHMENT
C     AND BE USED IN CORESSPONDANCE WITH Q0
C
          IF(NOBAND(HEAD,BAND).EQ.0.0) GOTO 240
            SBAR(HEAD,BAND)=-M*(ALOG(QINITL/Q0(HEAD,BAND)))
          QBAND=QINITL
C
C     ROUTING OUT THE INITIAL FLOWS IN THE SUBCATCHMENT WHERE
C     THE REFERENCE TIMESTEP IT HAS BEEN SET TO 0
C
          CALL ROUTE
  240   CONTINUE
  250 CONTINUE
C
      CLOSE (115)
      CLOSE (120)
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE PREAD
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     Using data file listed in PLYN.RUN
C
      DO 200 HEAD=1,NGAUGE
        I=15+HEAD-1
        READ(I,*)
        DO 100 IT=1,TSTART-1
          READ(I,*) NOWT
  100   CONTINUE
C       PRINT *,'Reading data input file',I,NOWT
        PRINT *
C
        DO 150 IT=TSTART,TEND
          READ(I,*) nowt,qobs(it,head),r(it,head),e(it,head)
  150   CONTINUE
```

```
  200 CONTINUE
C
      DO 50 I=15,16
        CLOSE(I)
   50 CONTINUE
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE TOPMOD
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      ITER=0
      NCALL=0
C
      IF (KOSTATUS.EQ.1) THEN
          OPEN(300,FILE='SBARV.DAT',STATUS='UNKNOWN')
      ELSEIF (KOSTATUS.EQ.2) THEN
          OPEN(300,FILE='SBARC.DAT',STATUS='UNKNOWN')
      ENDIF
C
C     WRITE VALUE OF GAMMA AND NT TO SBAR.DAT
      WRITE(300,10) NT,GAMMA(1,1)
   10 FORMAT(1X,'No. iterations =',I5,'; Gamma = ',F6.3)
C
      PRINT *,ALPHA,SK0
      PRINT *
      DO 500 IT=TSTART,TEND
       DO 400 HEAD=1,NHEAD
        DO 300 BAND=1,NBAND
C
C     HERE THE RUNNING TOTALS FOR EXCESS RUNOFF AND
C     UNSATURATED ZONE FLOWS ARE INITIALISED FOR EACH BAND
C
        ROFF=0.0
        QV=0.0
C
C     AVAILABLE AMOUNT OF WATER FOR INFILTRATION IS EQUAL
C     TO THE RAINFALL. IF AN INFILTRATION EXCESS ALGORITHM
C     IS USED THEN THE AMOUNT OF EXCESS IS DEDUCTED FROM THE
C     RAINFALL. HERE THE EXCESS IS SET EQUAL TO 0.0.
C     THE CALCULATION IS DONE FOR THE COMPLETE BAND.
C     THE EXCESS WILL ALREADY BE IN UNITS PER BAND
C
        IF(R(IT,HEAD).GE.0.0) THEN
          EX=0.0
          P=R(IT,HEAD)-EX
          IF(EX.GT.0.0) THEN
            ROFF=ROFF+EX
          ENDIF
        ELSE
          P=R(IT,HEAD)
        ENDIF
C
C       BEGIN ATB LOOP
C
        DO 200 ATB=1,MAX
C
          ITER=ITER+1
C
```

```
C         IF THERE IS NO AREA GO TO THE END OF THE ATB LOOP
          IF(NATB(HEAD,BAND,ATB).LE.0.0) GOTO 200
C
          S(HEAD,BAND,ATB)=SBAR(HEAD,BAND)+(M*(GAMMA(HEAD,BAND)-
     &                    A(ATB)))
          EX=0.0
          EX1=0.0
          EX2=0.0
          QUZ=0.0
C
C       IF S IS LESS THAN 0.0 THEN JUMP STRAIGHT TO THE
C       SATURATION EXCESS CALCULATIONS
          IF (S(HEAD,BAND,ATB).LT.0.0) GOTO 100
C
C       ROOT ZONE CALCULATIONS
C       EVAPOTRANSPORATION CONTINUES AT THE FULL RATE UNTIL THE
C       ROOT ZONE IS EMPTY
C
          SRZ(HEAD,BAND,ATB)=SRZ(HEAD,BAND,ATB)+P
          IF (SRZ(HEAD,BAND,ATB).GT.SRMAX) THEN
            SUZ(HEAD,BAND,ATB)=SUZ(HEAD,BAND,ATB)+
     &                        SRZ(HEAD,BAND,ATB)-SRMAX
            SRZ(HEAD,BAND,ATB)=SRMAX
          ENDIF
          EA=E(IT,HEAD)*(srz(head,band,atb)/srmax)
          SRZ(HEAD,BAND,ATB)=SRZ(HEAD,BAND,ATB)-EA
          SUBAE(HEAD)=SUBAE(HEAD)+(EA*NATB(HEAD,BAND,ATB)/
     &            NOHEAD(HEAD))
          ACAE=ACAE+(EA*NATB(HEAD,BAND,ATB)/TOTALA)
C
C       THE CASE OF SATURATION FROM ABOVE WHERE THE AMOUNT THAT
C       HAS GONE INTO THE GRAVITY DRAINAGE STORE EXCEEDS THE SPACE
C       AVAILABLE
C
          IF(SUZ(HEAD,BAND,ATB).GT.S(HEAD,BAND,ATB)) THEN
           EX=SUZ(HEAD,BAND,ATB)-S(HEAD,BAND,ATB)
           SUZ(HEAD,BAND,ATB)=S(HEAD,BAND,ATB)
           ROFF=ROFF+(EX*NATB(HEAD,BAND,ATB)/NOBAND(HEAD,BAND))
           SUBSU(HEAD)=SUBSU(HEAD)+(EX*NATB(HEAD,BAND,ATB)/
     &            NOHEAD(HEAD))
           ACSU=ACSU+(EX*NATB(HEAD,BAND,ATB)/TOTALA)
           EX1=EX
          ENDIF
C
C       UNSATURATED ZONE FLOWS WHICH IS SUMMED IN QV FOR THE
C       WHOLE BAND
C
          QUZ=ALPHA*SK0*(EXP(-S(HEAD,BAND,ATB)/M))
          IF(QUZ.LE.SUZ(HEAD,BAND,ATB))THEN
            WRITE(125,50)IT,HEAD,BAND,ATB,QUZ,SUZ(HEAD,BAND,ATB)
   50       FORMAT(1X,I4,2I2,I3,2F7.4)
          ELSE
            QUZ=SUZ(HEAD,BAND,ATB)
          ENDIF
          QV=QV+(QUZ*NATB(HEAD,BAND,ATB)/NOBAND(HEAD,BAND))
          SUBQV(HEAD)=SUBQV(HEAD)+(QUZ*NATB(HEAD,BAND,ATB)/
     &            NOHEAD(HEAD))
          ACQV=ACQV+(QUZ*NATB(HEAD,BAND,ATB)/TOTALA)
          SUZ(HEAD,BAND,ATB)=SUZ(HEAD,BAND,ATB)-QUZ
C
C         SKIP OVER THE SATURATED AREA CALCULATIONS
C
          GOTO 150
C
```

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C          THE CASE FOR SATURATED AREAS
  100      CONTINUE
           EX=0.0
           SRZ(HEAD,BAND,ATB)=SRZ(HEAD,BAND,ATB)+P
           IF(SRZ(HEAD,BAND,ATB).GT.SRMAX) THEN
              SUZ(HEAD,BAND,ATB)=SUZ(HEAD,BAND,ATB)+
     &                           SRZ(HEAD,BAND,ATB)-SRMAX
              SRZ(HEAD,BAND,ATB)=SRMAX
           ENDIF
           EX=SUZ(HEAD,BAND,ATB)
           SUZ(HEAD,BAND,ATB)=0.0
           IF(EX.GT.0.0) THEN
            ROFF=ROFF+(EX*NATB(HEAD,BAND,ATB)/NOBAND(HEAD,BAND))
            SUBSE(HEAD)=SUBSE(HEAD)+(EX*NATB(HEAD,BAND,ATB)/
     &                  NOHEAD(HEAD))
            ACSE=ACSE+(EX*NATB(HEAD,BAND,ATB)/TOTALA)
            EX2=EX
           ENDIF
           EA=E(IT,HEAD)*(srz(head,band,atb)/srmax)
           SRZ(HEAD,BAND,ATB)=SRZ(HEAD,BAND,ATB)-EA
           SUBAE(HEAD)=SUBAE(HEAD)+(EA*NATB(HEAD,BAND,ATB)/
     &                 NOHEAD(HEAD))
           ACAE=ACAE+(EA*NATB(HEAD,BAND,ATB)/TOTALA)
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
  150      IF((EX.LE.0.0).AND.(QUZ.LE.0.0)) GOTO 200
C
C        ENDING THE ATB LOOP
C
  200    CONTINUE
C
C        IF THERE ARE NO CELLS IN THE BAND, GO TO THE END OF THE BAND
C        LOOP
C
         IF(NOBAND(HEAD,BAND).GT.0.0) THEN
C
C          CALCULATE THE BASEFLOW FOR THE WHOLE BAND AND THEN
C          PASS IT AND THE ROFF VALUE TO BE ROUTED
C          QB IS IN UNITS PER BAND
C
           QB=Q0(HEAD,BAND)*(EXP(-SBAR(HEAD,BAND)/M))
           SUBQB(HEAD)=SUBQB(HEAD)+(QB*NOBAND(HEAD,BAND)/NOHEAD(HEAD))
           ACQB=ACQB+(QB*NOBAND(HEAD,BAND)/TOTALA)
           QBAND=QB+ROFF
C
           CALL ROUTE
C
           SBAR(HEAD,BAND)=SBAR(HEAD,BAND)+QB-QV
         ENDIF
C
C        ENDING THE BAND LOOP
C
  300    CONTINUE
C
C       ENDING THE HEAD LOOP
C
  400   CONTINUE
C
C      WRITE IT AND SBAR TO SEPARATE FILE FOR MAPPING OF SMD VALUES
       WRITE (300,*) IT,SBAR(1,1)
C
```

```
C     ENDING THE TIMESTEP LOOP
C
  500 CONTINUE
C     CLOSE(300)
C
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE ROUTE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      IF(HEAD.NE.1) THEN
C
C     IF THERE IS MORE THAN 1 SUBCATCHMENT
C
C     ROUTING TO AN INTERNAL GAUGE FOR ALL SUBCATCHMENTS ABOVE
C     THE OUTFLOW SUBCATCHMENT
C
        DELAY=IT+INT(((DIST(BAND)-GAUGE(HEAD))/CHV))
C
C       If there is only 1 area/distance band for each headwater,
C       then DELAY = IT and QHEAD = QBAND
C
        IF(DELAY.NE.0) THEN
C
C         QBAND IS CONVERTED TO FLOW PER UNIT HEADWATER
C
          QHEAD=QBAND*(NOBAND(HEAD,BAND)/NOHEAD(HEAD))
          Q(DELAY,HEAD)=Q(DELAY,HEAD)+QHEAD
        ENDIF
C
      ELSE
C
C     IF THERE IS ONLY 1 CATCHMENT....
C
C     ROUTING TO OUTFALL (eg. GAUGE(1)=0.0 metres), AND
C     CONVERTING TO FLOW PER UNIT AREA FOR ALL THE CATCHMENT
C
C     QALL = contribution of the given QBAND to tot. catchment flow
        QALL=QBAND*NOBAND(HEAD,BAND)/TOTALA
        DELAY=IT+INT((DIST(BAND)/CHV))
        IF(DELAY.NE.0) THEN
          Q(DELAY,1)=Q(DELAY,1)+QALL
        ENDIF
C
      ENDIF
C
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE RESULTS
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      DO 30 HEAD=1,NHEAD
```

```
        IF(KOSTATUS.EQ.1)THEN
          WRITE((20+HEAD),1) m,SRMAX,SOILFILE
    1     FORMAT(1X,' m = ',F6.4,', SRMAX = ',F6.4,', KO = ',A)
        ELSE
          WRITE((20+HEAD),2) m,SRMAX
    2     FORMAT(1X,' m = ',F6.4,', SRMAX = ',F6.4,', KO = constant')
        ENDIF
        WRITE((20+HEAD),3) HEAD
    3   FORMAT(1X,' SUBCATCHMENT ',I1)
        WRITE((20+HEAD),5)
    5   FORMAT(1X,'   IT      Qcalc        Qobs         R         E')
        DO 20 IT=TSTART,TEND
          SUMOBS(HEAD)=SUMOBS(HEAD)+QOBS(IT,HEAD)
          SUMSIM(HEAD)=SUMSIM(HEAD)+Q(IT,HEAD)
          SUMR(HEAD)=SUMR(HEAD)+R(IT,HEAD)
          SUME(HEAD)=SUME(HEAD)+E(IT,HEAD)
          WRITE((20+HEAD),10) IT,Q(IT,HEAD),QOBS(IT,HEAD),
     &                        R(IT,HEAD),E(IT,HEAD)
   10     FORMAT(1X,I5,2F11.8,2F9.6)
   20   CONTINUE
   30 CONTINUE
C
      CLOSE(21)
      CLOSE(22)
C
      RETURN
      END
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE WATBAL
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      INCLUDE 'COMMON.FOR'
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     THE TOTAL AMOUNT OF WATER REMAINING IN THE STORES IS SUMMED
C     FOR THE WHOLE CATCHMENT
C
      REAL QBPCT,QSEPCT,QSAPCT,SUMRZ,SUMUZ
C
      BAND=0
      DO 30 HEAD=1,NHEAD
         BAND=BAND+1
C
         ENSBAR=ENSBAR+(SBAR(HEAD,BAND)*NOBAND(HEAD,BAND)/TOTALA)
         SUMRZ=0.0
         SUMUZ=0.0
         WRITE(125,5)HEAD,BAND
    5    FORMAT(/,1X,'HEAD = ',I3,/
     &            1X,'BAND = ',I3,/
     &            1X,'   ATB   SRZ     SUZ     SUMRZ    SUMUZ',//)
         DO 10 ATB=1,MAX
           SUMRZ=SUMRZ + SRZ(HEAD,BAND,ATB)*NATB(HEAD,BAND,ATB)/
     &          TOTALA
           SUMUZ=SUMUZ + SUZ(HEAD,BAND,ATB)*NATB(HEAD,BAND,ATB)/
     &          TOTALA
           WRITE(125,6) ATB,SRZ(HEAD,BAND,ATB),SUZ(HEAD,BAND,ATB),
     &                  SUMRZ,SUMUZ
    6      FORMAT(1X,I5,4F8.6)

   10    CONTINUE
         BALEND=BALEND+SUMRZ+SUMUZ
         WRITE(125,*) 'BALEND = ', BALEND
```

```
C
   30 CONTINUE
C
C     N.B. The final water balance can only be calculated for the
C     entire catchment, if using BALINI, ALSBAR, etc.that are also
C     calculated for the entire catchment...
      BUDGET(1)=SUMR(1)-ACAE-SUMSIM(1)-(BALINI-BALEND)-
     &         (ALSBAR-ENSBAR)
C
      IF(KOSTATUS.EQ.2) THEN
        WRITE(30,901)M,SRMAX,SK0,T0
  901   FORMAT(3(1x,1F16.6/),1x,1F16.6)
      ELSE
        WRITE(30,902)M,SRMAX,SK0,MEANT0(1)
  902   FORMAT(3(1x,1F16.6/),1x,1F16.6)
      ENDIF

C     BEGIN SUBCATCHMENT LOOP
C
      BAND=0
      DO 75 HEAD=1,NHEAD
         BAND=BAND+1
C
         IF(NHEAD.GT.1) THEN
          IF(K0STATUS.EQ.2)THEN
           WRITE(30,906) HEAD,T0
  906      FORMAT(1X,'***** SUBCATCHMENT ',I3,' *****',/,
     &            1X,1F16.6)
          ELSE
           WRITE(30,911) HEAD,MEANT0(HEAD)
  911      FORMAT(1X,'***** SUBCATCHMENT ',I3,' *****',/,
     &            1X,1F16.6)
          ENDIF
         ENDIF
C
C        CALCULATING THE EFFICIENCY OF THE MODEL
C
         QOBAR(HEAD)=SUMOBS(HEAD)/NT
         PRINT*,'QOBAR(HEAD)=',QOBAR(HEAD)
         DO 50 IT=TSTART,TEND
           SSE(HEAD)=SSE(HEAD)+((QOBS(IT,HEAD)-Q(IT,HEAD))**2)
           VARI(HEAD)=VARI(HEAD)+((QOBS(IT,HEAD)-QOBAR(HEAD))**2)
   50    CONTINUE
         EFF(HEAD)=(1-(SSE(HEAD)/VARI(HEAD)))*100
         PRINT*,'SSE(HEAD)=',SSE(HEAD)
         PRINT*,'VAR(HEAD)=',VARI(HEAD)
         WRITE(*,921) HEAD,EFF(HEAD)
  921    FORMAT(1X,'Efficiency catchment no. ',I2,' = ',1F6.2,'%',/)
C
   75 CONTINUE
C
C     BREAKDOWN OF FLOW COMPONENTS FOR ENTIRE CATCHMENT
C     Calculate % of each flow component...
C
      QBPCT=(ACQB/SUMOBS(1))*100
      QSEPCT=(ACSE/SUMOBS(1))*100
      QSAPCT=(ACSU/SUMOBS(1))*100
C
C     write catchment results to excel file...
C
     write(30,950)ACAE,SUMSIM(1),ACQV,ACQB,QBPCT,ACSE,QSEPCT,ACSU,
    &             QSAPCT
  950 FORMAT(/1X,'************ CATCHMENT SUMMARY ***********',//
     &       3(1x,1F16.6/),
```

```
     &        3(1x,1f10.6,' / ',1f6.2/)/)
      WRITE(30,960)ALSBAR,ENSBAR,BALINI,BALEND,BUDGET(1)
  960 FORMAT(/1X,'************ CATCHMENT SUMMARY ***********',/
     &         5(1x,1F9.3/))
C
      CLOSE(30)
      CLOSE(125)
      CLOSE(200)
      RETURN
      END
```

C) Soil Moisture Deficit Program

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      PROGRAM SMDERR
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     PROGRAM TO CALCULATE SMD(X,Y) MAPS AND DIFFERENCES IN SOIL
C     MOISTURE DEFICIT MAPS DERIVED USING 2 DIFFERENT SOIL
C     CLASSIFICATIONS
C
C     PROCEDURE
C      1) load two different SBAR files (eg. const K0 vs HOST SPR)
C      2) define two diff. smd arrays: smd1(x,y) & smd2(x,y)
C      3) input soil type values into separate array (X,Y,soil-id)
C         [X,Y can be diff from x,y as long as NX,NY are known]
C      4) calculate SMD(X,Y) maps for each soil classification
C      4) calculate smd diff. on cell by cell basis
C      5) calculate average diff per soil type
C      6) calculate catchment total smd difference
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      INTEGER NT1,NT2,NX,NY,NCOL,NROW,SIZE,TSTART,TEND,FLAG,T,
     &        DELTAX,DELTAY,X,Y,XCOORD,YCOORD,XLL,XUL,YLL,YUL,
     &        COUNT1,COUNT2,COUNT(6),EVENT
C
      REAL SBAR1,SBAR2,M,GAMMA1,GAMMA2,ATOB(76,82),SMD,
     &     SMD1(76,82),SMD2(76,82),DIFFSMD(76,82),AVGDIFF,
     &     DELTASMD(6),AVGDELTA(6),SUMDIFF,SOIL, EVNTERR(8760),
     &     SOILERR(6,8760)
C
      CHARACTER*12 NAME1,NAME2,NAME3
      CHARACTER*15 PARAMS$
      CHARACTER*80 TITLE
C
C     LOAD ALL INPUT DATA FILES FROM "PLYN.RUN" FILE
      OPEN(1000,FILE="PLYN.RUN",STATUS="OLD")
C
      READ(1000,"(A)")TITLE
      READ(1000,"(A)")PARAMS$
      READ(1000,*)
      READ(1000,*)
      READ(1000,*)
      READ(1000,*) K0STATUS
C
      OPEN(5,FILE=PARAMS$,STATUS="OLD")
      OPEN(10,FILE='GRID.DAT',STATUS="OLD")
C
C     READING IN THE CONTROL PARAMETERS
C
      READ(5,*)
      READ(5,*) M,SRMAX,SK0,ALPHA,CHV
      READ(10,*) NX,NY
C
C     READING IN COORDINATE REFERENCE DATA
C
      OPEN(UNIT=30,FILE='UPHODTM.DAT',STATUS='OLD',FORM='FORMATTED')
C
      read(30,20)ncol
      read(30,20)nrow
      read(30,25)xll
      read(30,25)yll
```

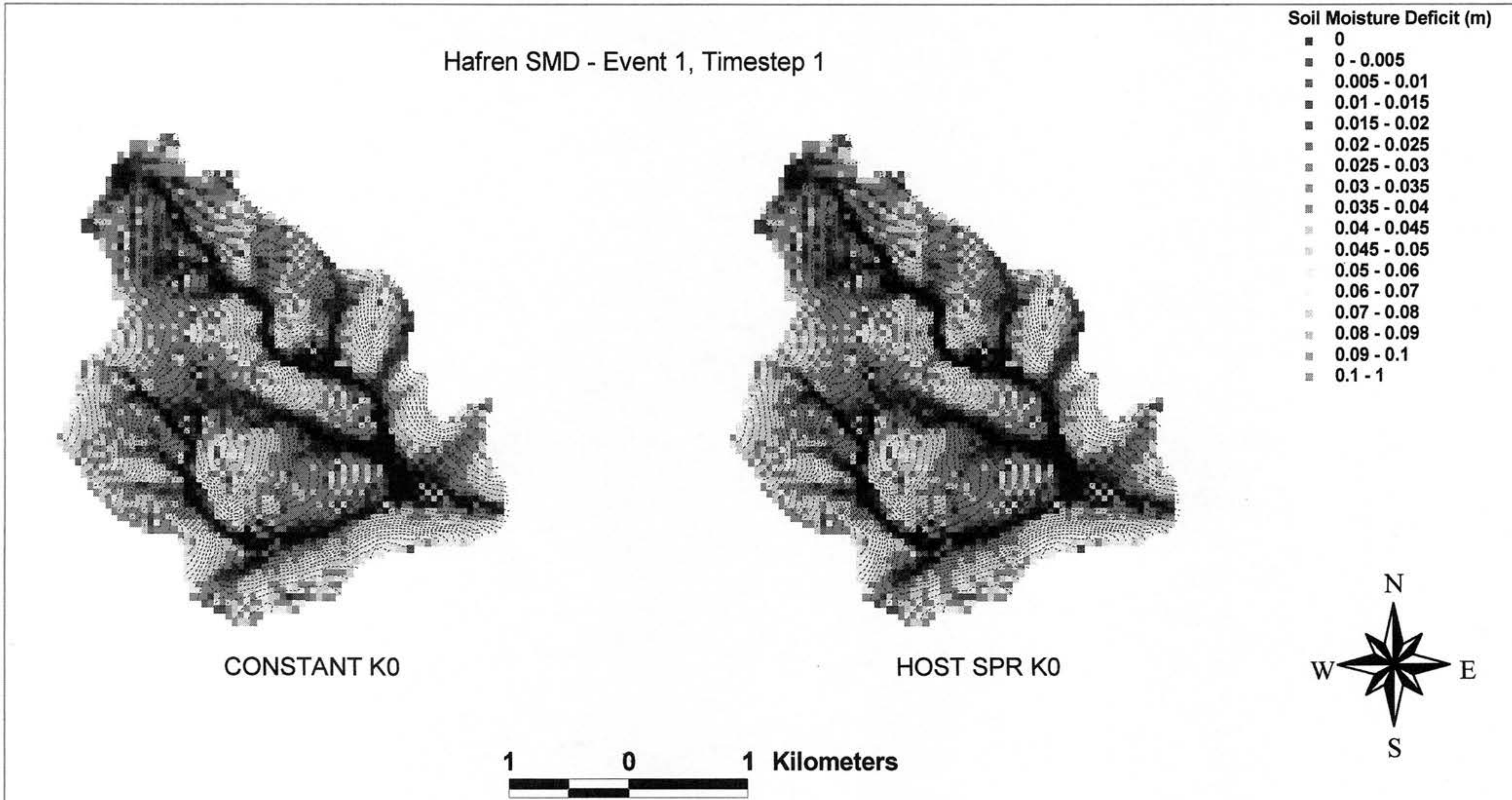
```
      read(30,20)size
C     read(30,20)null
      deltax=(ncol)*size
      deltay=(nrow)*size
      xul=xll
      yul=yll+deltay
      write(*,30)ncol,nrow,size,xll,yll,xul,yul,deltax,deltay
C
   20 format(14x,i6)
   25 format(14x,i6)
   30 format(1x,'No. of columns = ',i5,/
     &       1x,'No. of rows    = ',i5,/
     &       1x,'Cell Size      = ',i5,/
     &       1x,'DEM (xll,yll)  = ',2i10,/
     &       1x,'DEM (xul,yul)  = ',2i10,/
     &       1x,'Delta X (m)    = ',i10,/
     &       1x,'Delta Y (m)    = ',i10,/)
C
C     Opening SBAR input and output files
C
 5000 OPEN(35,FILE='SBAR_PV.DAT',STATUS="UNKNOWN")
      READ(35,40) NT1,GAMMA1
      PRINT *,NT1,GAMMA1
      OPEN(36,FILE='SBAR_PC.DAT',STATUS="UNKNOWN")
      READ(36,40) NT2,GAMMA2
      PRINT *, NT2,GAMMA2
   40 FORMAT(17X,I5,9X,F6.3)
C     PRINT *,NT,GAMMA
C
      PRINT*,'**********************************************'
      PRINT*,'ARE YOU USING THE CORRECT YFREEATB & ATOB FILE???'
      PRINT*,'**********************************************'
      PRINT*
C
C     Calc. of smd errors is required for multiple timesteps
C     - define no. of IT values
C     - loop to read IT and SBAR values
C     - loop to calculate deficit maps
C
      PRINT *,'Type in event no.'
      READ (*,*) EVENT
C
      PRINT *,'Type in value of start timestep'
      READ (*,*) TSTART
      PRINT *,'Type in value of end timestep'
      READ (*,*) TEND
C
C     INITIALISE ARRAYS & VARIABLES
C
 6000 DO 60 Y=1,NY
       DO 50 X=1,NX
         SMD1(X,Y)=0.0
         SMD2(X,Y)=0.0
         DIFFSMD(X,Y)=0.0
   50  CONTINUE
   60 CONTINUE
      COUNT1=0
      COUNT2=0
C
C     READ IN SBAR DATA...
C
    5 FLAG=9
      READ(35,*) T,SBAR1
      READ(36,*) T,SBAR2
```

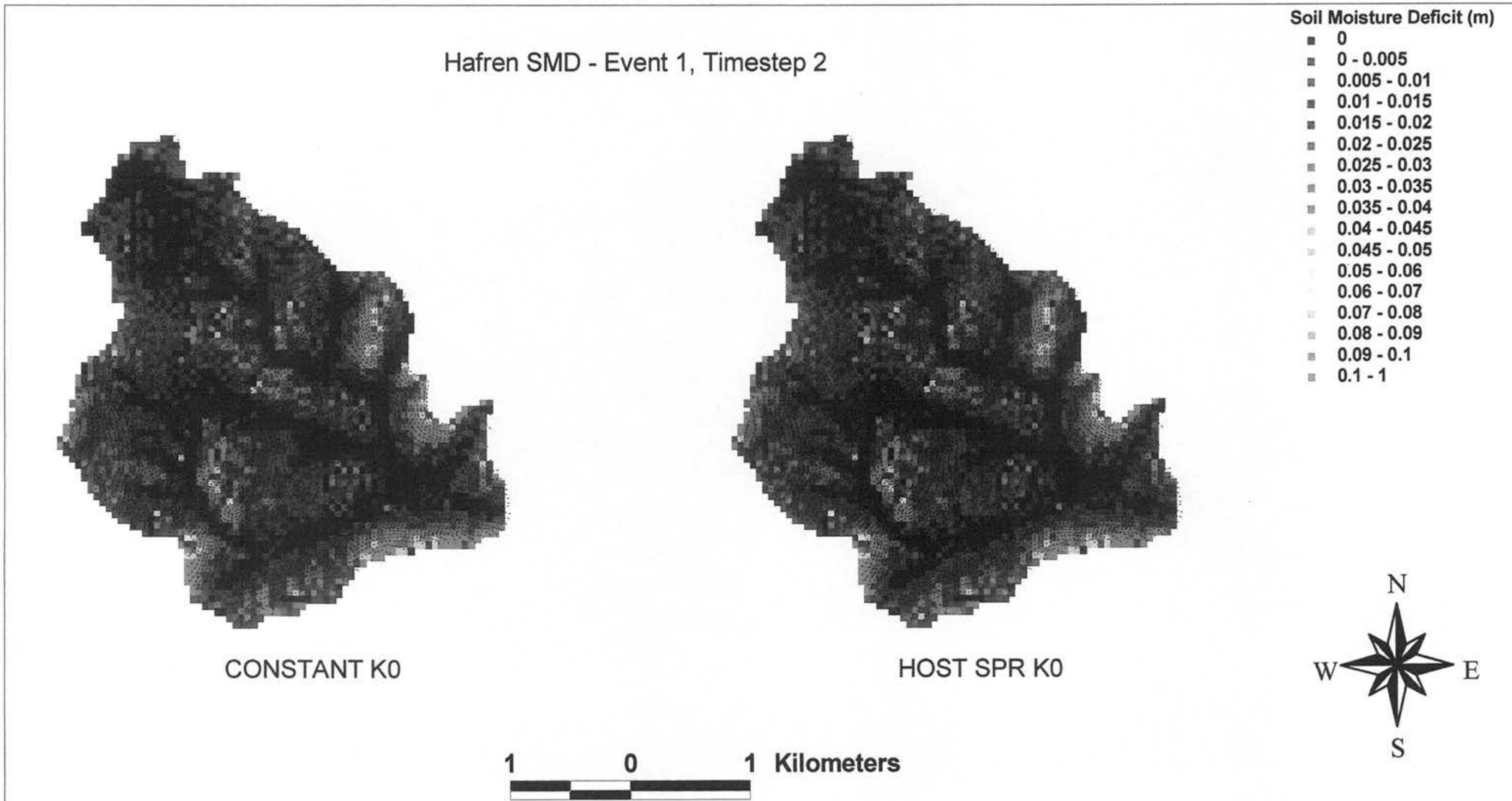
```
      IF((T.GE.TSTART).AND.(T.LE.TEND)) THEN
        FLAG=-9
      ENDIF
      IF(FLAG.NE.-9)GOTO 5
C
C     CALCULATING SMD FOR FIRST SOIL DISTRIBUTION (VARIABLE K0)
C
        OPEN(40,FILE='SMD1.DAT',STATUS='UNKNOWN')
        OPEN(50,FILE='ATOB.DAT',STATUS='OLD')
        READ(50,*)
C
        DO 500 Y=1,NY
          DO 400 X=1,NX
            READ(50,*)I,J,ATOB(X,Y)
C           READ(40,*) I,J,SMD
            IF(ATOB(X,Y).LT.2990) THEN
               COUNT1=COUNT1+1
               SMD1(X,Y)=SBAR1+M*(GAMMA1-ATOB(X,Y))
C              SMD1(X,Y)=SMD
               IF(SMD1(X,Y).LE.0.0) SMD1(X,Y)=0.0
C
            ELSE
               SMD1(X,Y)=-999
            ENDIF
C           CONVERT X,Y COORDS TO NAT.GRID COORDS
            XCOORD=XUL+(X-1)*SIZE
            YCOORD=YUL-(Y-1)*SIZE
            WRITE(40,300)XCOORD,YCOORD,SMD1(X,Y)
  300       FORMAT(1X,I7,',',I7,',',F12.6)
  400     CONTINUE
  500   CONTINUE
C
C     CALCULATING SMD FOR SECOND DISTRIBUTION (CONSTANT K0)
C

        OPEN(60,FILE='SMD2.DAT',STATUS='UNKNOWN')
        OPEN(70,FILE='YFREEATB.DAT',STATUS='OLD')
        READ(70,*)
        T0=M*SK0
C
        DO 900 Y=1,NY
          DO 800 X=1,NX
            READ(60,*)I,J,SMD
            READ(70,*)I,J,ATOB(X,Y)
            IF(ATOB(X,Y).LT.2990) THEN
               COUNT2=COUNT2+1
               ATOB(X,Y)=ATOB(X,Y)-ALOG(T0)
               SMD2(X,Y)=SBAR2+M*(GAMMA2-ATOB(X,Y))
               IF(SMD2(X,Y).LE.0.0) SMD2(X,Y)=0.0
            ELSE
               SMD2(X,Y)=-999
            ENDIF
C           CONVERT X,Y COORDS TO NAT.GRID COORDS
            XCOORD=XUL+(X-1)*SIZE
            YCOORD=YUL-(Y-1)*SIZE
            WRITE(60,700)XCOORD,YCOORD,SMD2(X,Y)
  700       FORMAT(1X,I7,',',I7,',',F12.6)
  800     CONTINUE
  900   CONTINUE

C
C     N.B. DIFFSMD FILES MUST BE WRITTEN OUT FOR EACH TIMESTEP
C
      SUMDIFF = 0.0
```

```
      DO 950 I=1,6
         DELTASMD(I)=0
         COUNT(I)=0
         AVGDELTA(I)=0
  950 CONTINUE
C
C     SIMPLE DATA VALIDATION
C
      IF(COUNT1.NE.COUNT2) THEN
        PRINT *,' CHECK DATA  !'
      ENDIF
C
      OPEN(75,FILE='DIFFSMD.DAT',STATUS='UNKNOWN')
      OPEN(80,FILE='SOIL50MP.DAT',STATUS='OLD')
C
C     CALCULATE SMD DIFFERENCES
C
      DO 1200 Y=1,NY
        DO 1100 X=1,NX
          READ(80,*)I,J,SOIL
          COUNT(SOIL)=COUNT(SOIL)+1
C
C         -IF SMD1 <0 OR SMD2 <0, THE CELL DOES NOT HAVE A
C          DIFFSMD VALUE
C         -IF BOTH SMD1 AND SMD2 ARE = 0, THE FOLLOWING METHOD
C          ASSIGNS THE DIFFERENCE EQUAL TO ZERO
          IF((SMD1(X,Y).LT.0.0).OR.(SMD2(X,Y).LE.0.0)) THEN
             DIFFSMD(X,Y)= -9.0
          ELSEIF ((SMD1(X,Y).EQ.0.0).AND.(SMD2(X,Y).EQ.0.0)) THEN
             DIFFSMD(X,Y)= 0.0
          ELSE
             DIFFSMD(X,Y) = SMD1(X,Y)-SMD2(X,Y)
             SUMDIFF = SUMDIFF + DIFFSMD(X,Y)
             DELTASMD(SOIL)=DELTASMD(SOIL)+DIFFSMD(X,Y)
          ENDIF
          IF(SMD2(X,Y).NE.-999) THEN
             DIFFSMD(X,Y)=SMD1(X,Y)-SMD2(X,Y)
             SUMDIFF = SUMDIFF + DIFFSMD(X,Y)
             DELTASMD(SOIL)=DELTASMD(SOIL)+DIFFSMD(X,Y)
          ENDIF
          XCOORD=XUL+(X-1)*SIZE
          YCOORD=YUL-(Y-1)*SIZE
          WRITE(75,1000)X,Y,DIFFSMD(X,Y),SOIL
 1000     FORMAT(1X,I7,',',I7,',',F12.6,',',F5.1)
 1100   CONTINUE
 1200 CONTINUE
C
C     OPEN SUMMARY OUTPUT FILES...
C
      WRITE(NAME1,'(A7,I1,A4)') 'EVNTSUM',EVENT,'.TXT'
      WRITE(NAME2,'(A7,I1,A4)') 'SOILSUM',EVENT,'.TXT'
      WRITE(NAME3,'(A7,I1,A4)') 'SOILTYP',EVENT,'.TXT'
C
      OPEN(100,FILE=NAME1,STATUS="UNKNOWN")
      OPEN(110,FILE=NAME2,STATUS="UNKNOWN")
      OPEN(120,FILE=NAME3,STATUS="UNKNOWN")
C
C     CALCULATE AVG. SMD ERROR FOR INDIVIDUAL TIMESTEP
      AVGDIFF = SUMDIFF/COUNT1
      WRITE (100, 1220)T,AVGDIFF
 1220 FORMAT(1X,i5,f13.9)
C
C     CALCULATE AVG. SMD ERROR FOR EACH SOIL TYPE
      DO 1300 I=1,6
```

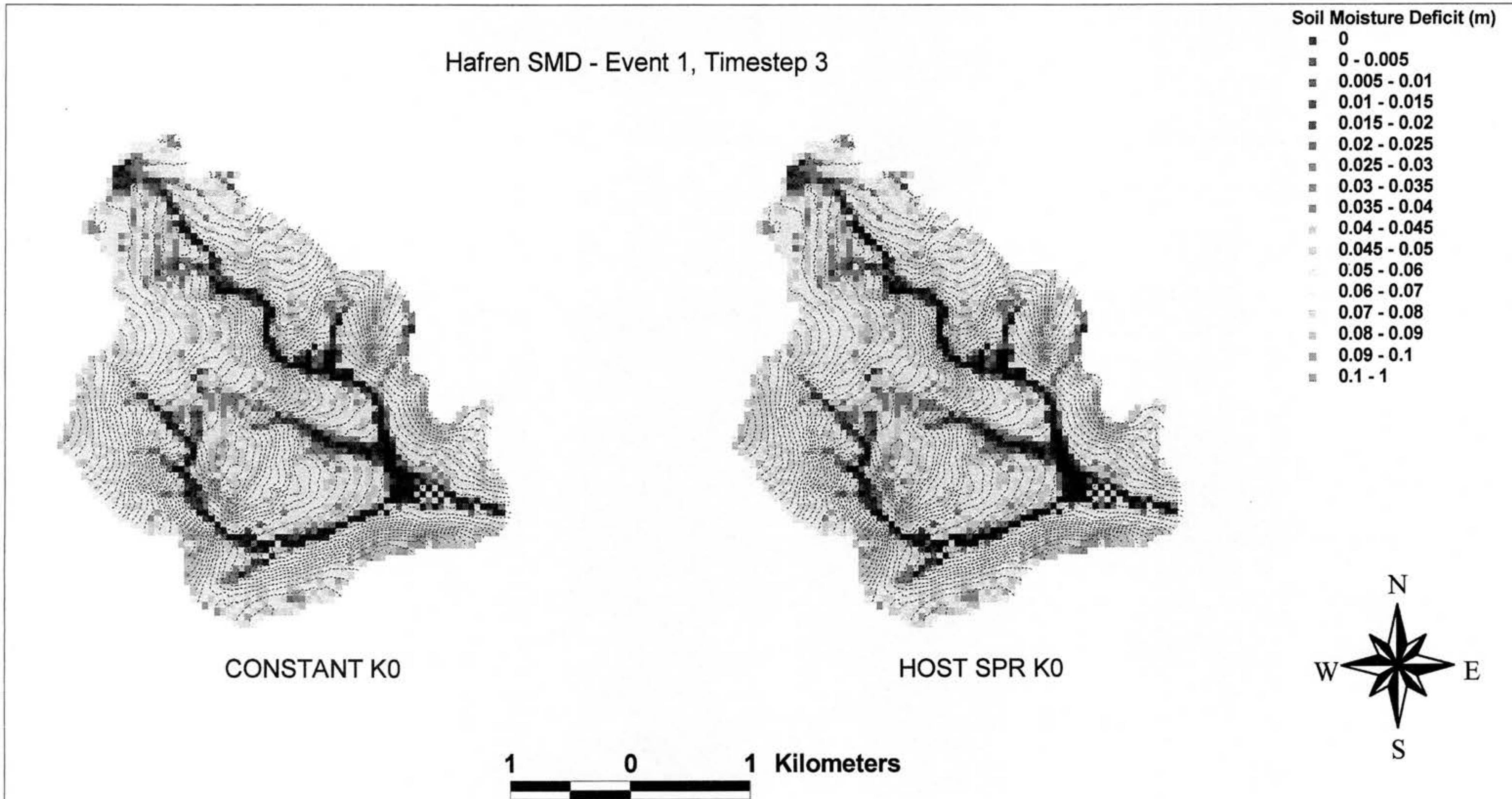
```
          AVGDELTA(I)=DELTASMD(I)/COUNT(I)
 1300 CONTINUE
      WRITE (110, 1290) T,AVGDELTA
      WRITE (120, 1290) T,DELTASMD
 1290 FORMAT(1X,i4,6f8.5)
      CLOSE(40)
      CLOSE(45)
      CLOSE(50)
      CLOSE(60)
C
      IF((T+1).LE.TEND) GOTO 6000
C
      CLOSE(35)
      CLOSE(36)
      CLOSE(100)
      CLOSE(110)
      CLOSE(120)
 7000 END
```

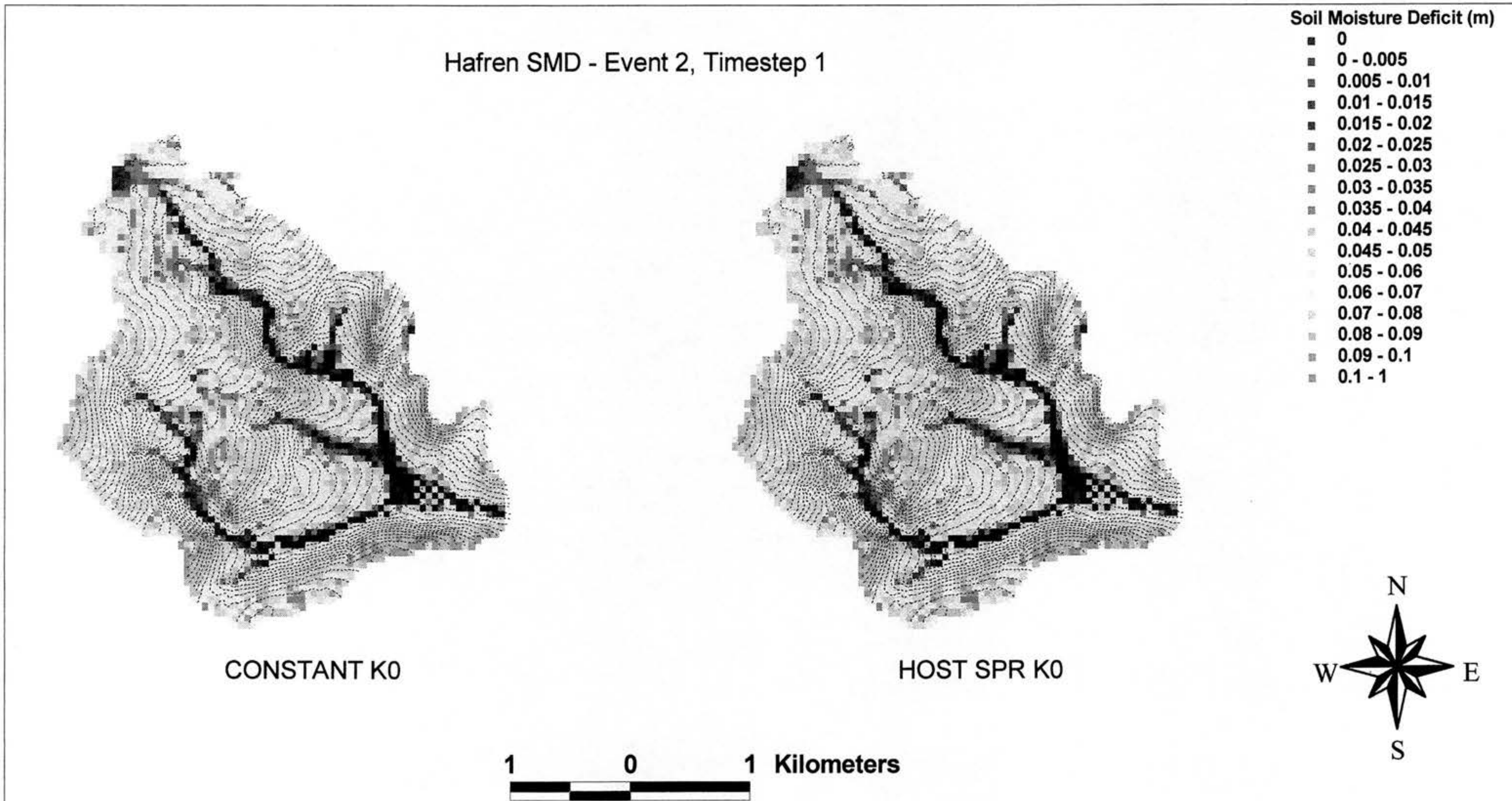
Appendix 2

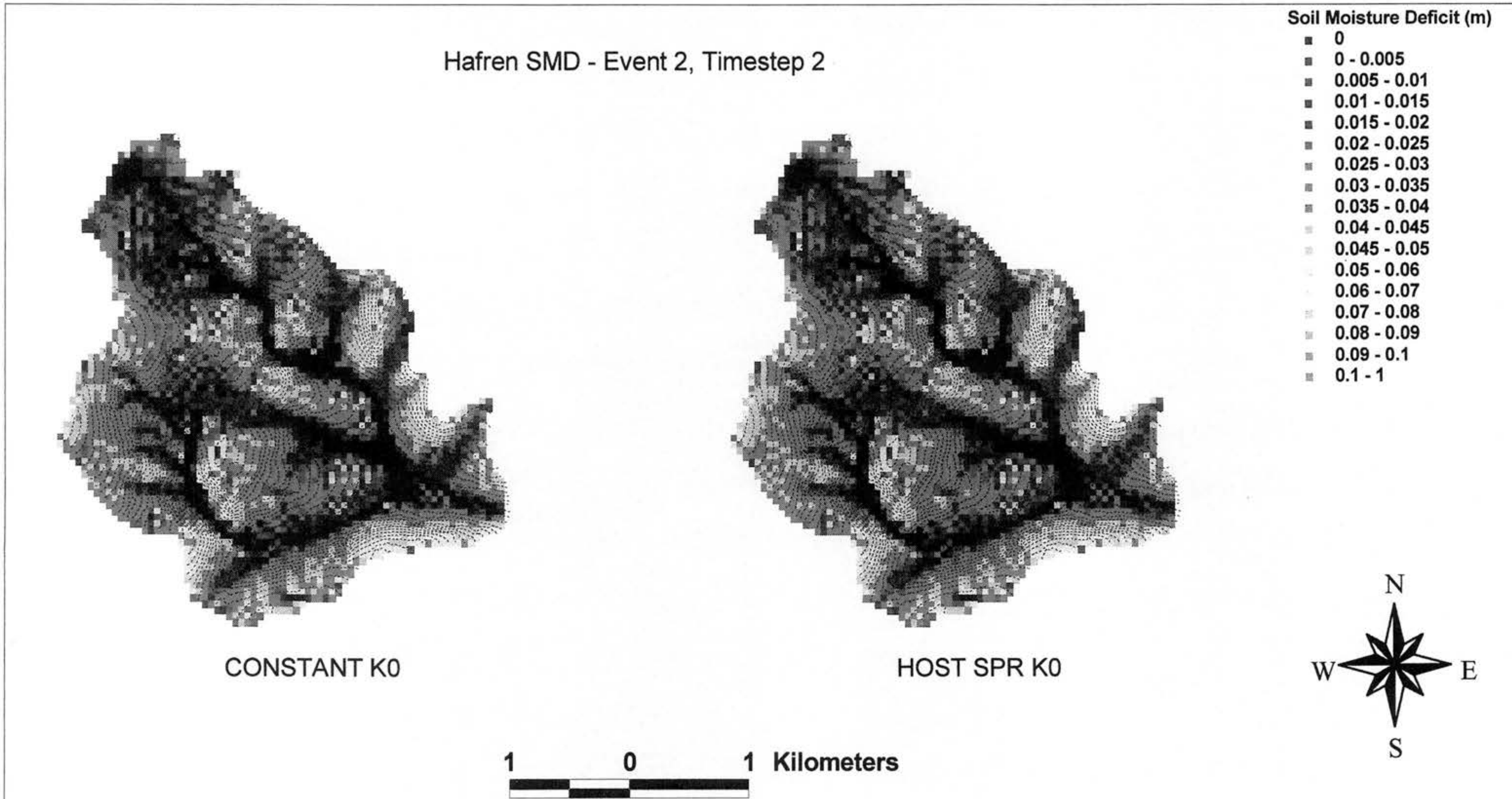

Hafren SMD - Event 1, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1 0 1 Kilometers

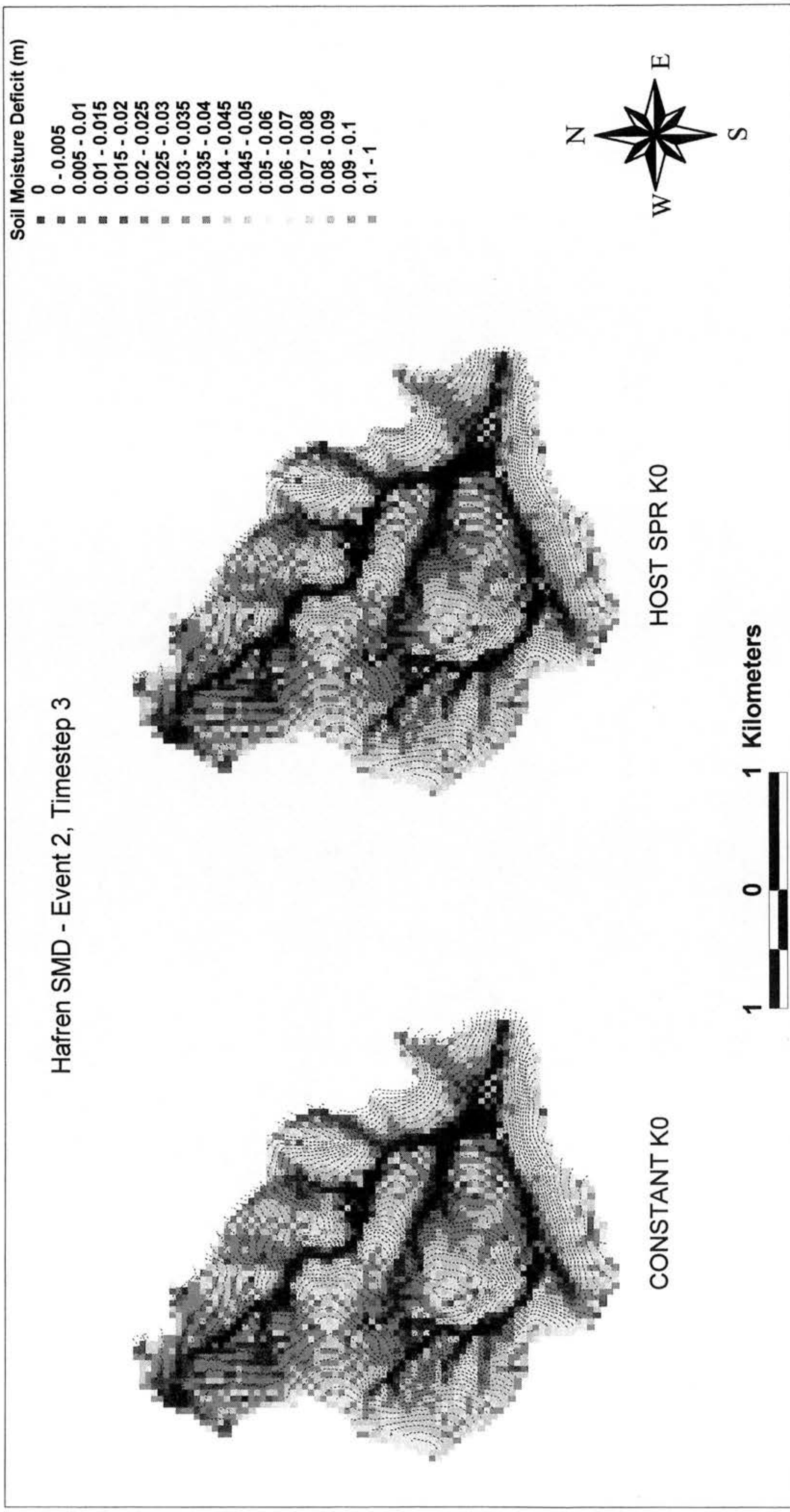


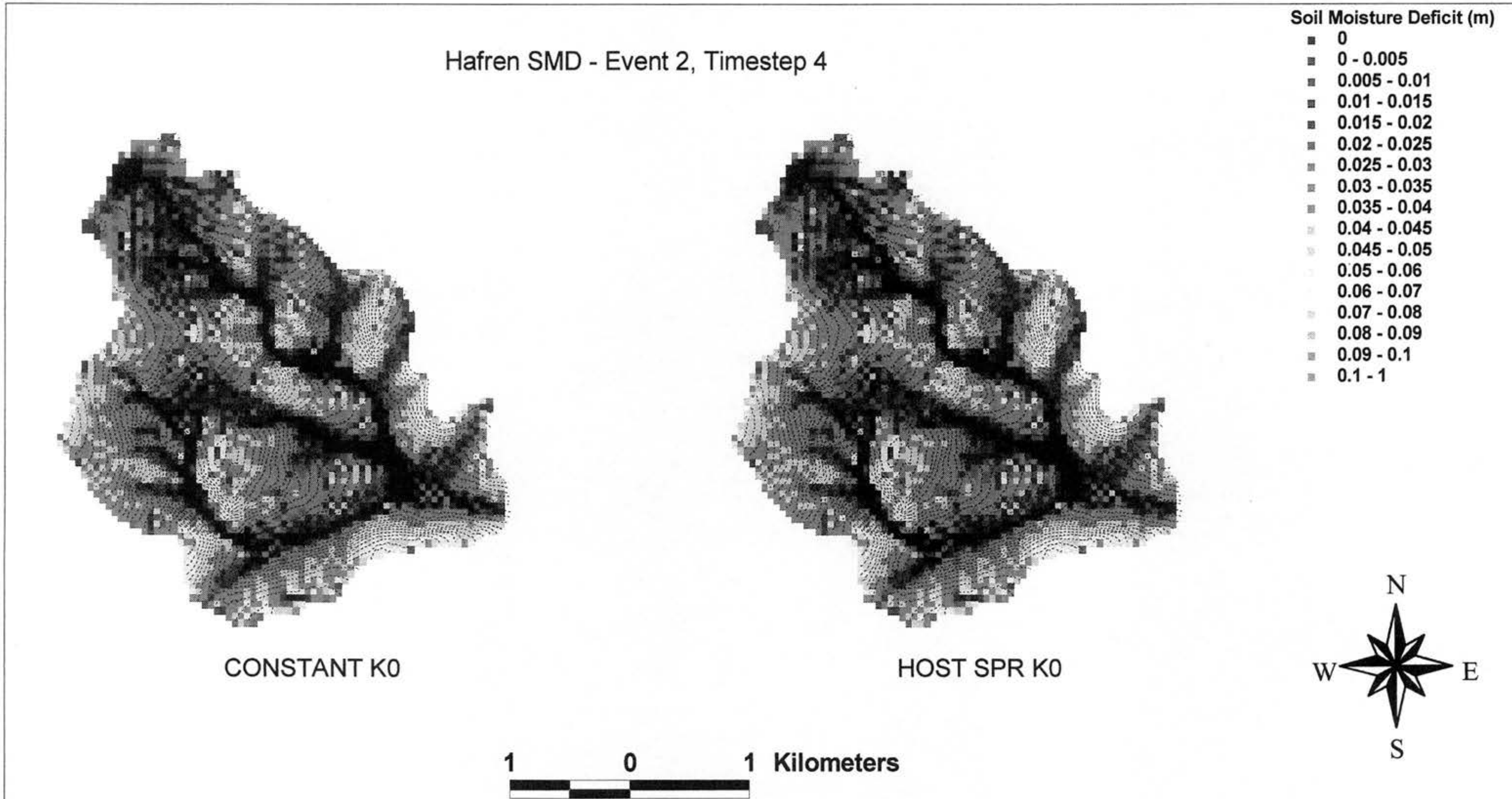
Hafren SMD - Event 1, Timestep 2
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1 0 1 Kilometers

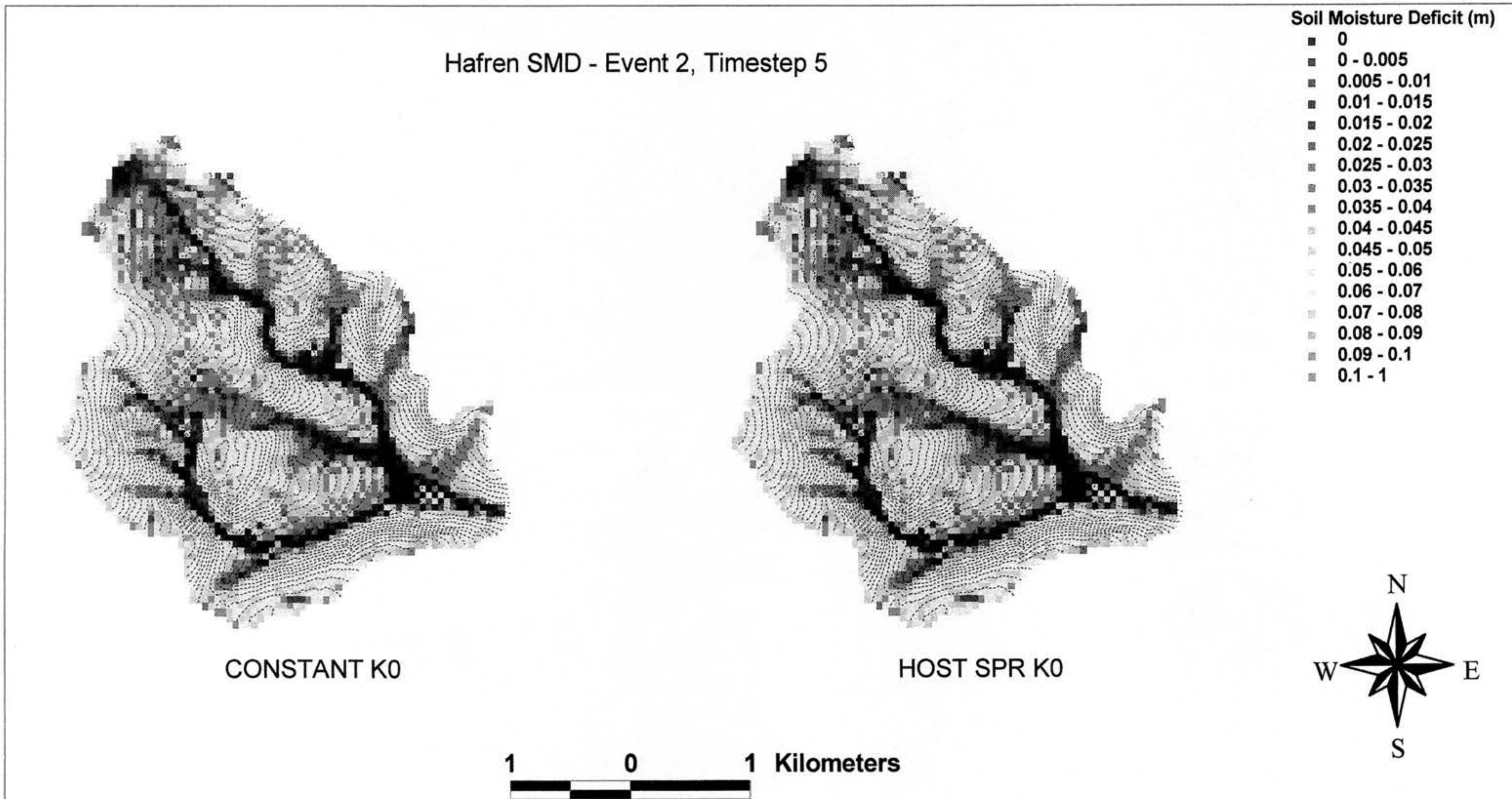

Hafren SMD - Event 1, Timestep 3
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

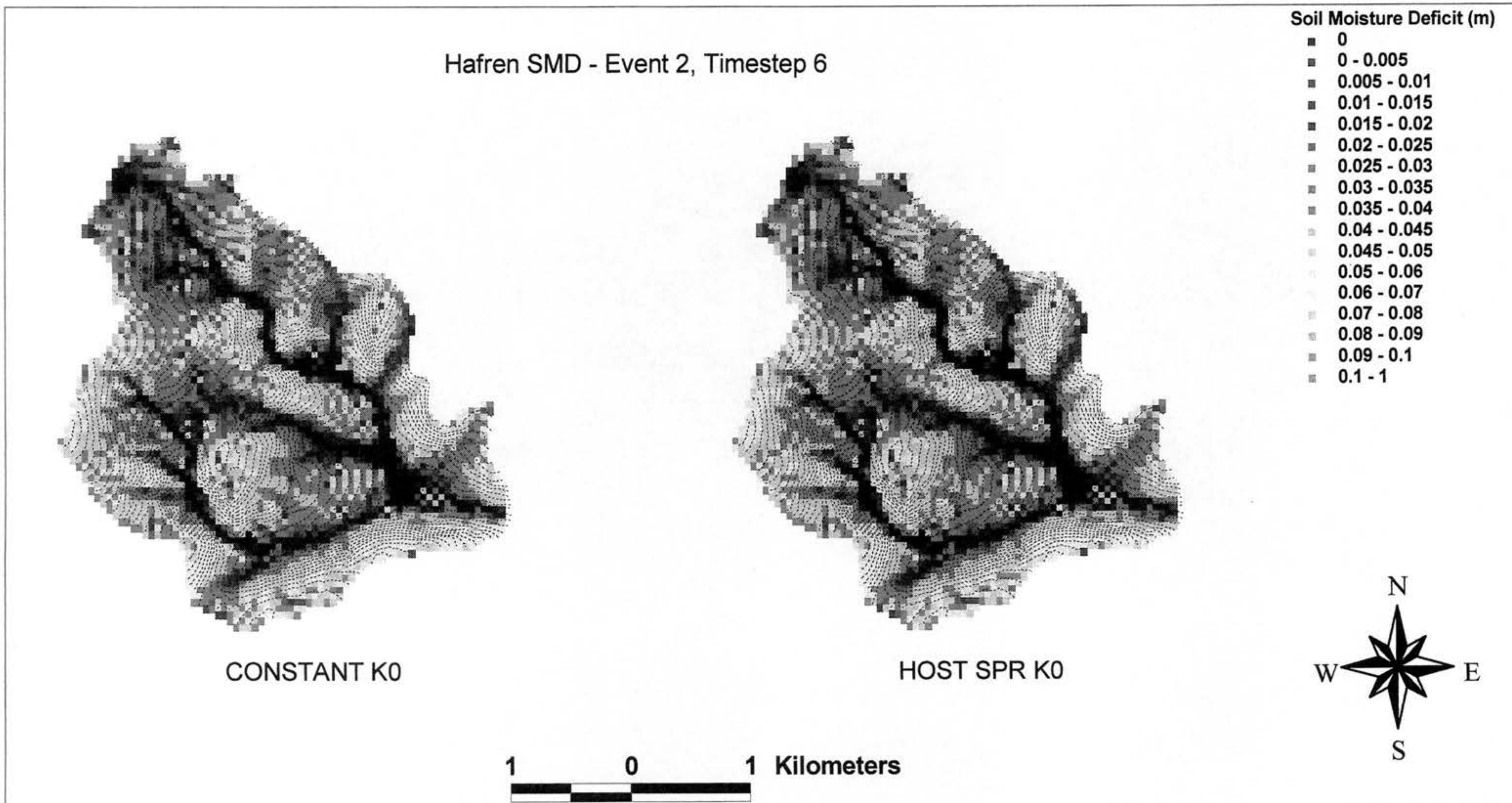

Hafren SMD - Event 2, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

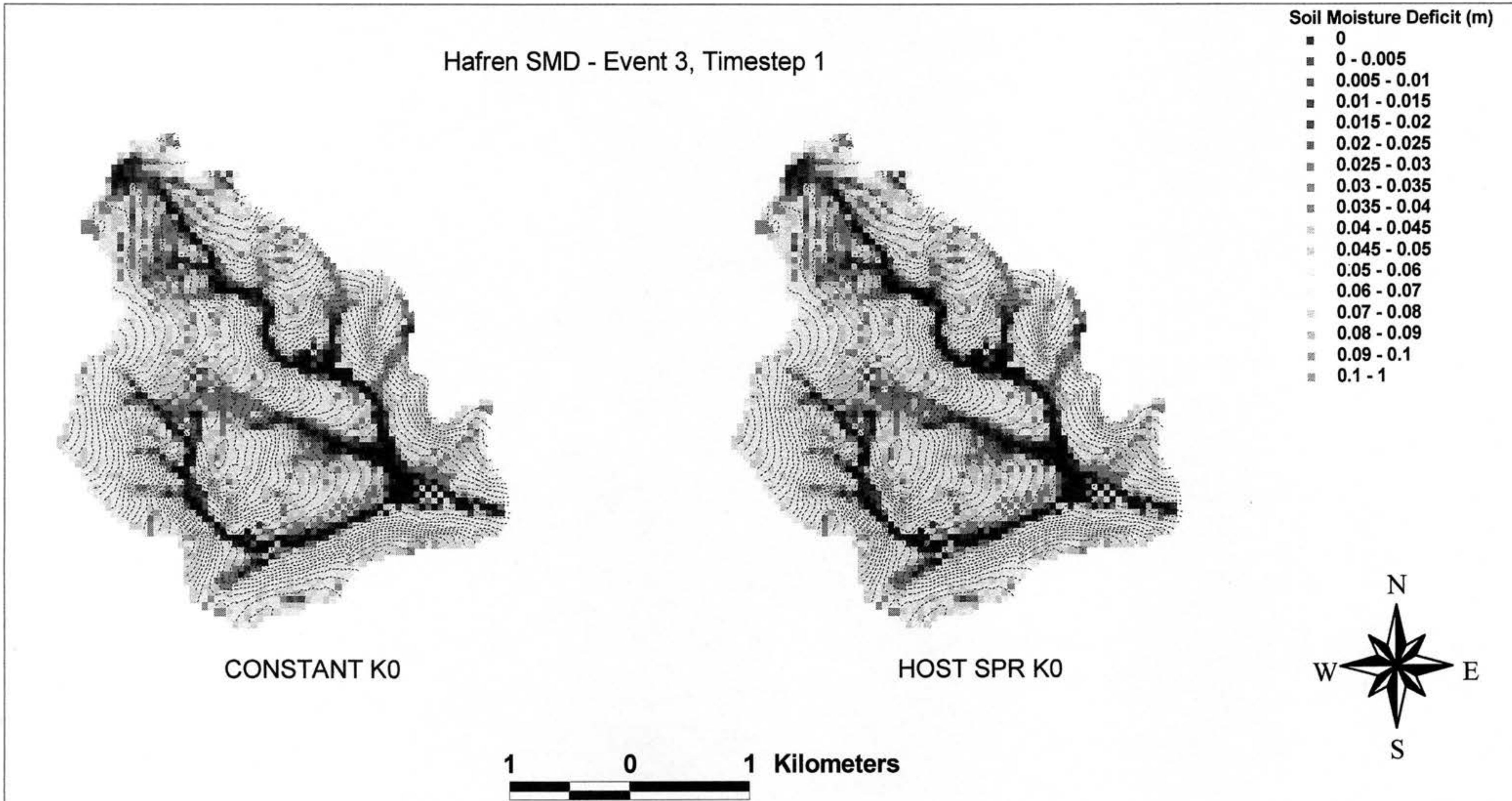

Hafren SMD - Event 2, Timestep 2
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1 0 1 Kilometers


Hafren SMD - Event 2, Timestep 3
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
N
E
S
W
CONSTANT K0
HOST SPR K0
1
0
1
Kilometers

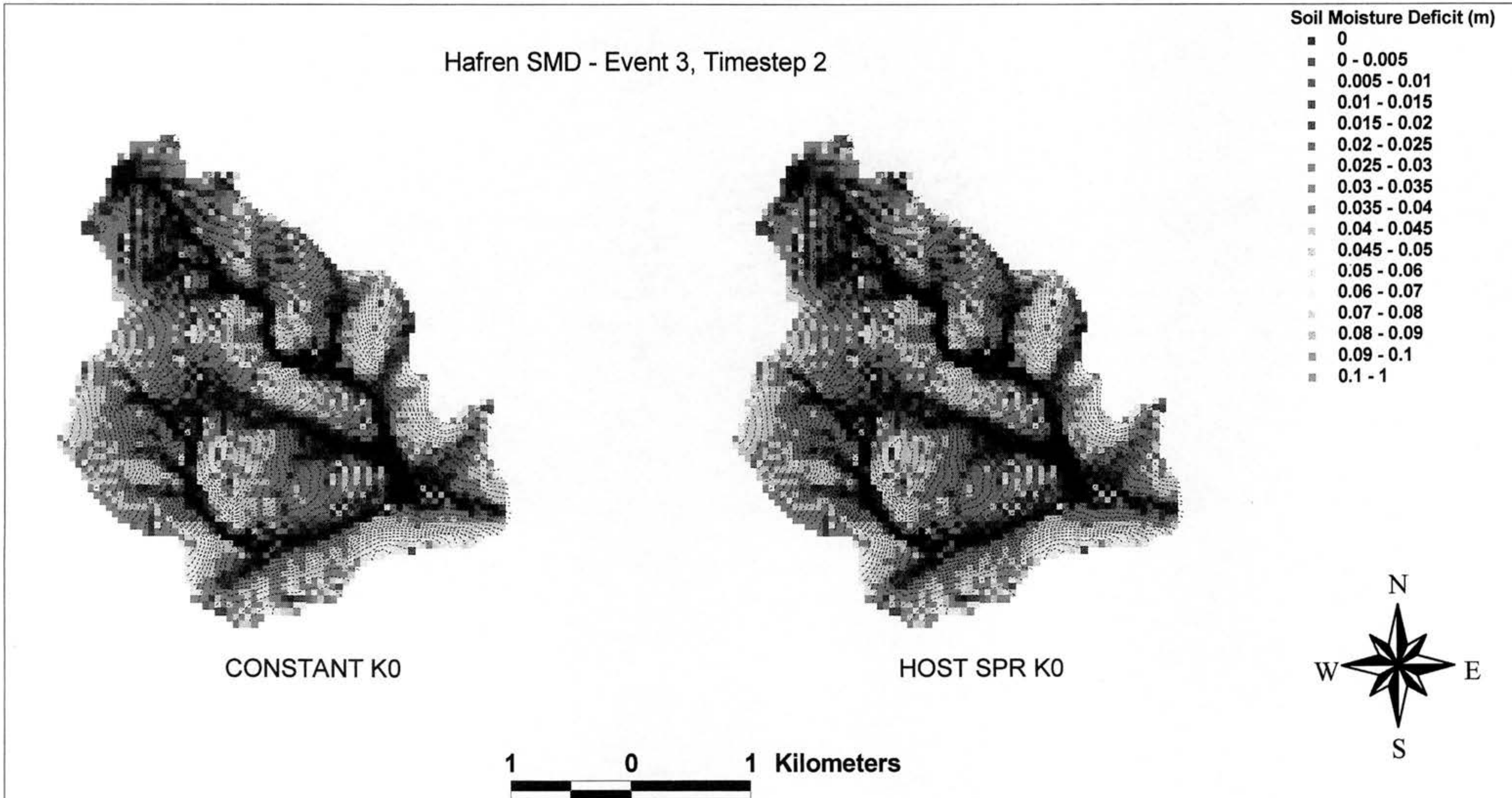

Hafren SMD - Event 2, Timestep 4
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

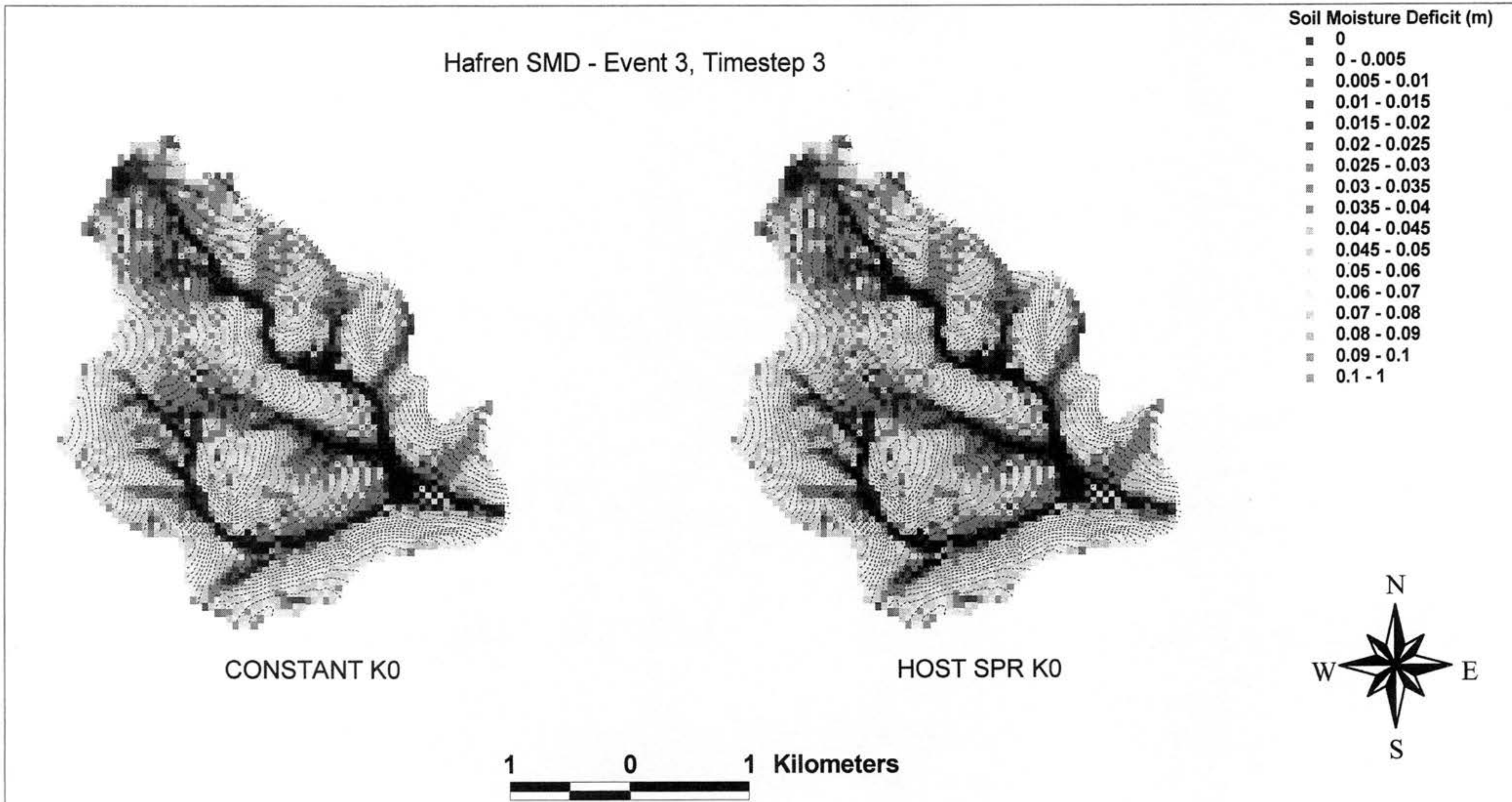

Hafren SMD - Event 2, Timestep 5
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

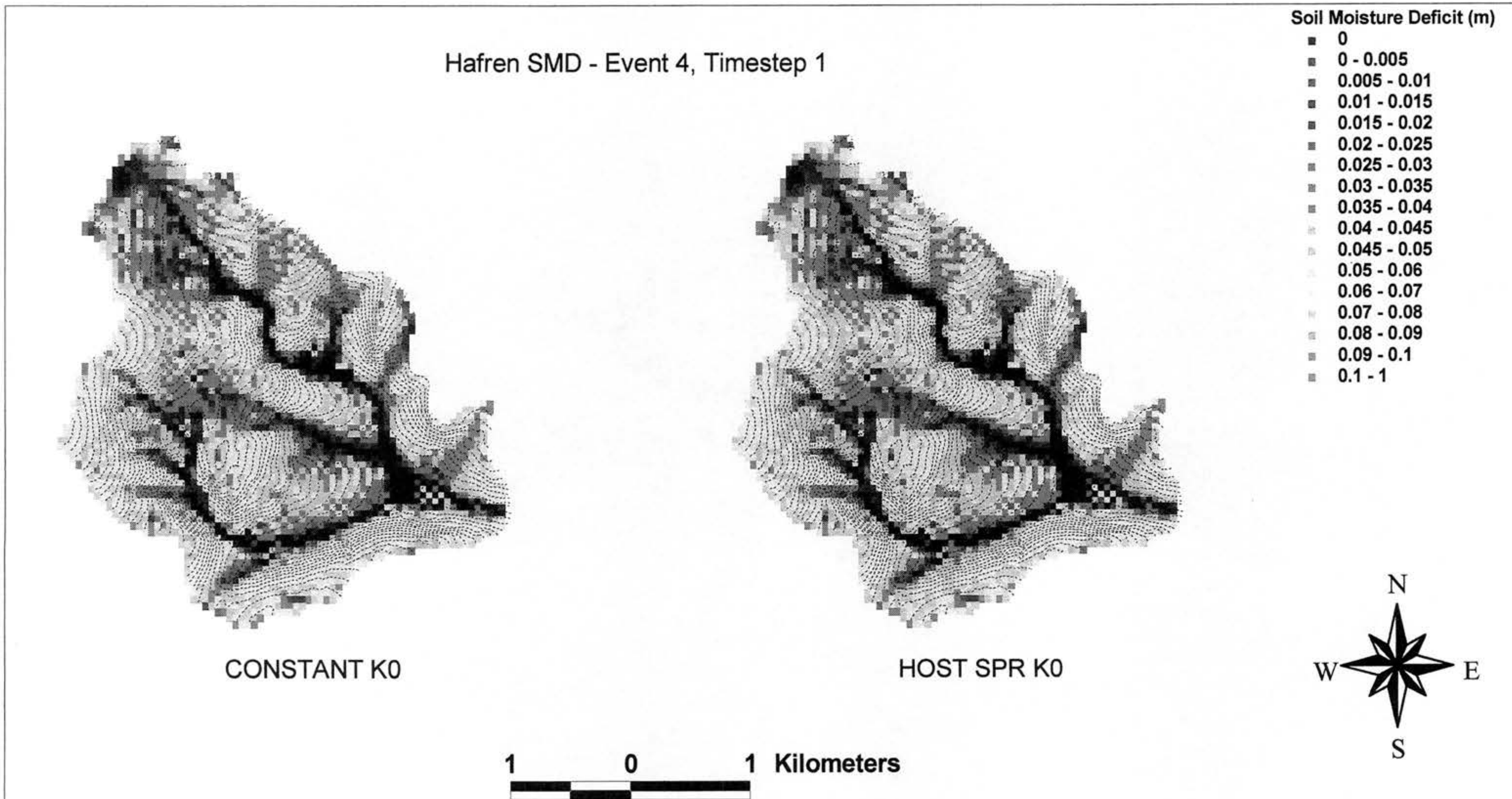

Hafren SMD - Event 2, Timestep 6
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers



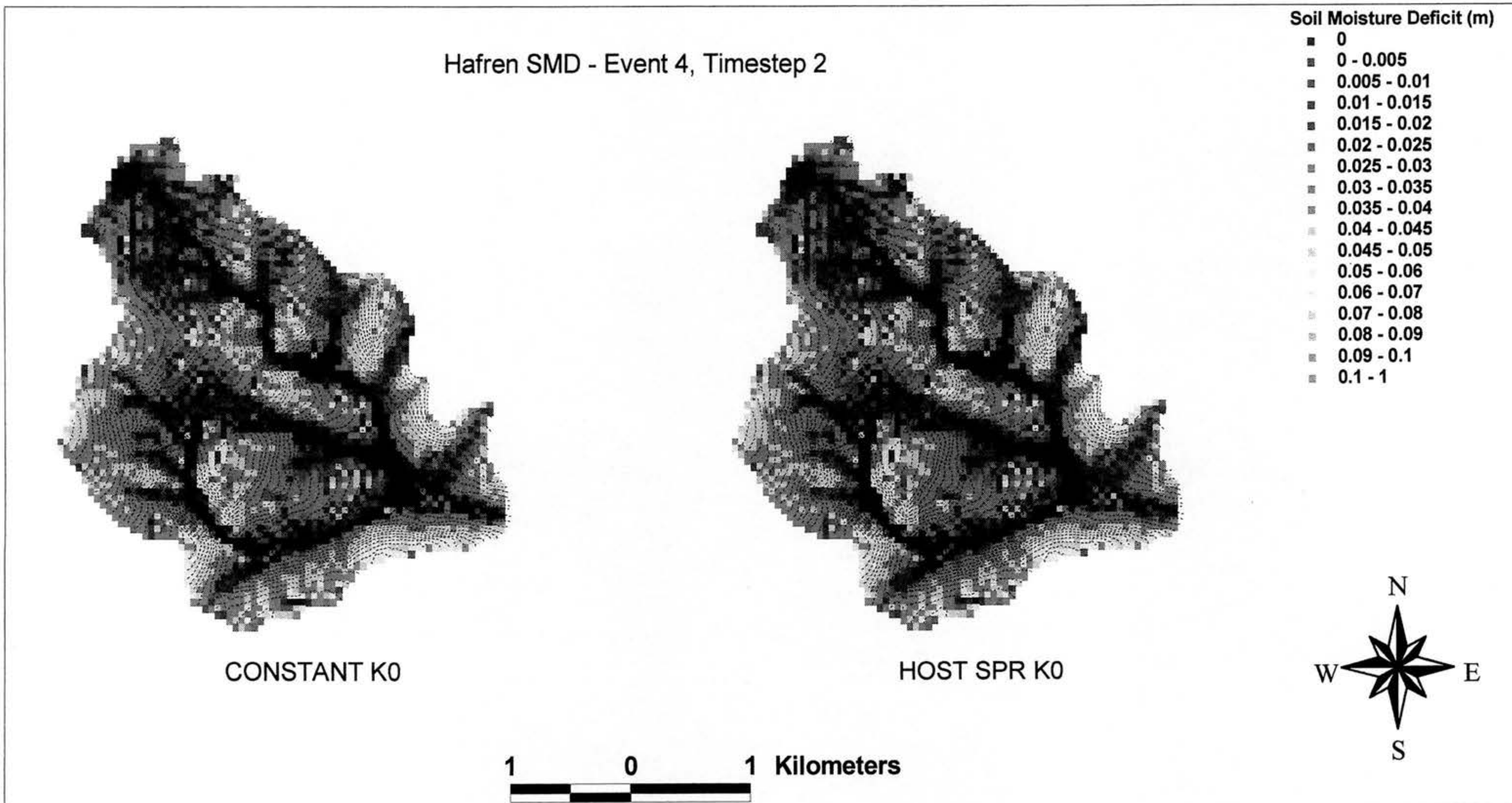
Hafren SMD - Event 3, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

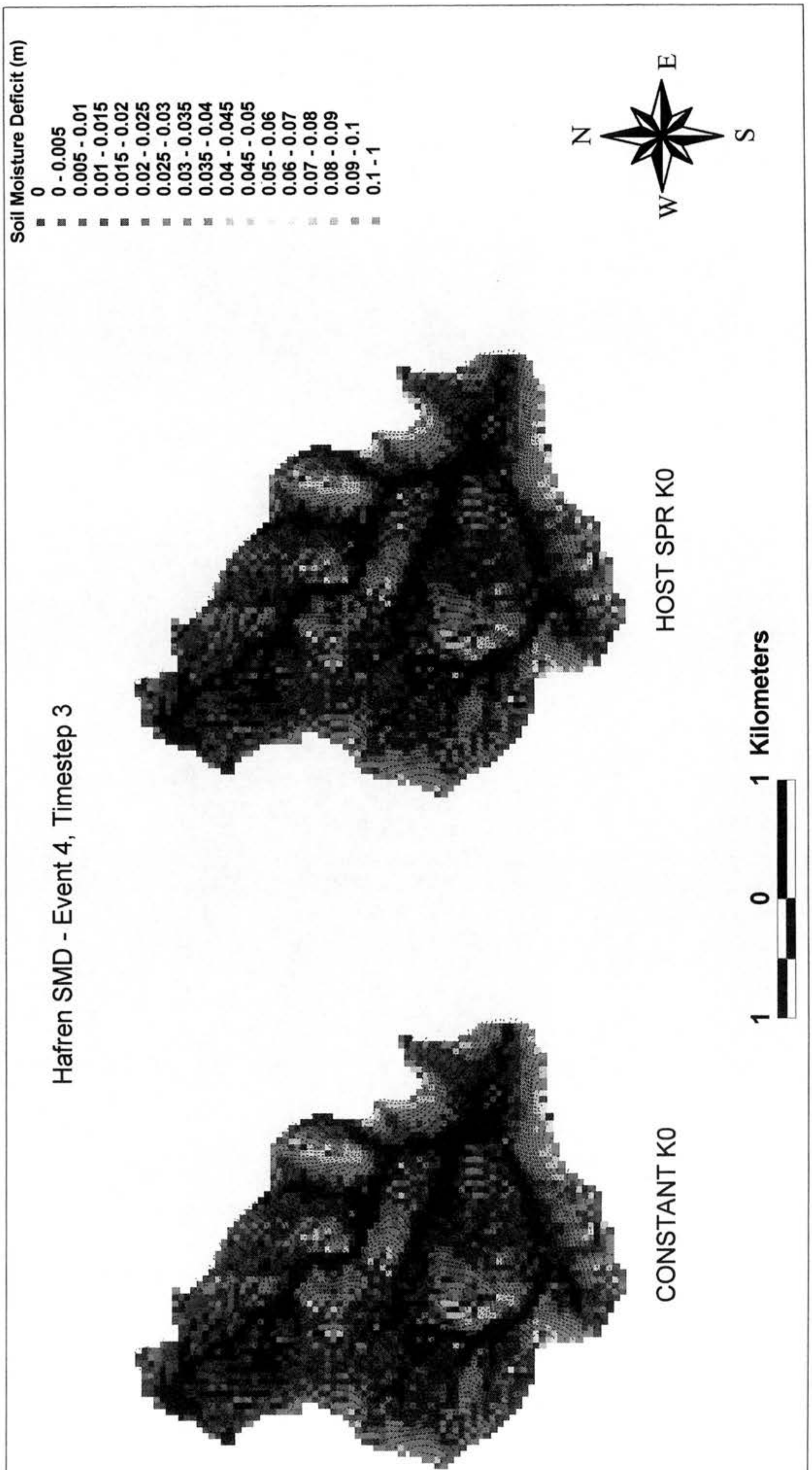

Hafren SMD - Event 3, Timestep 2
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

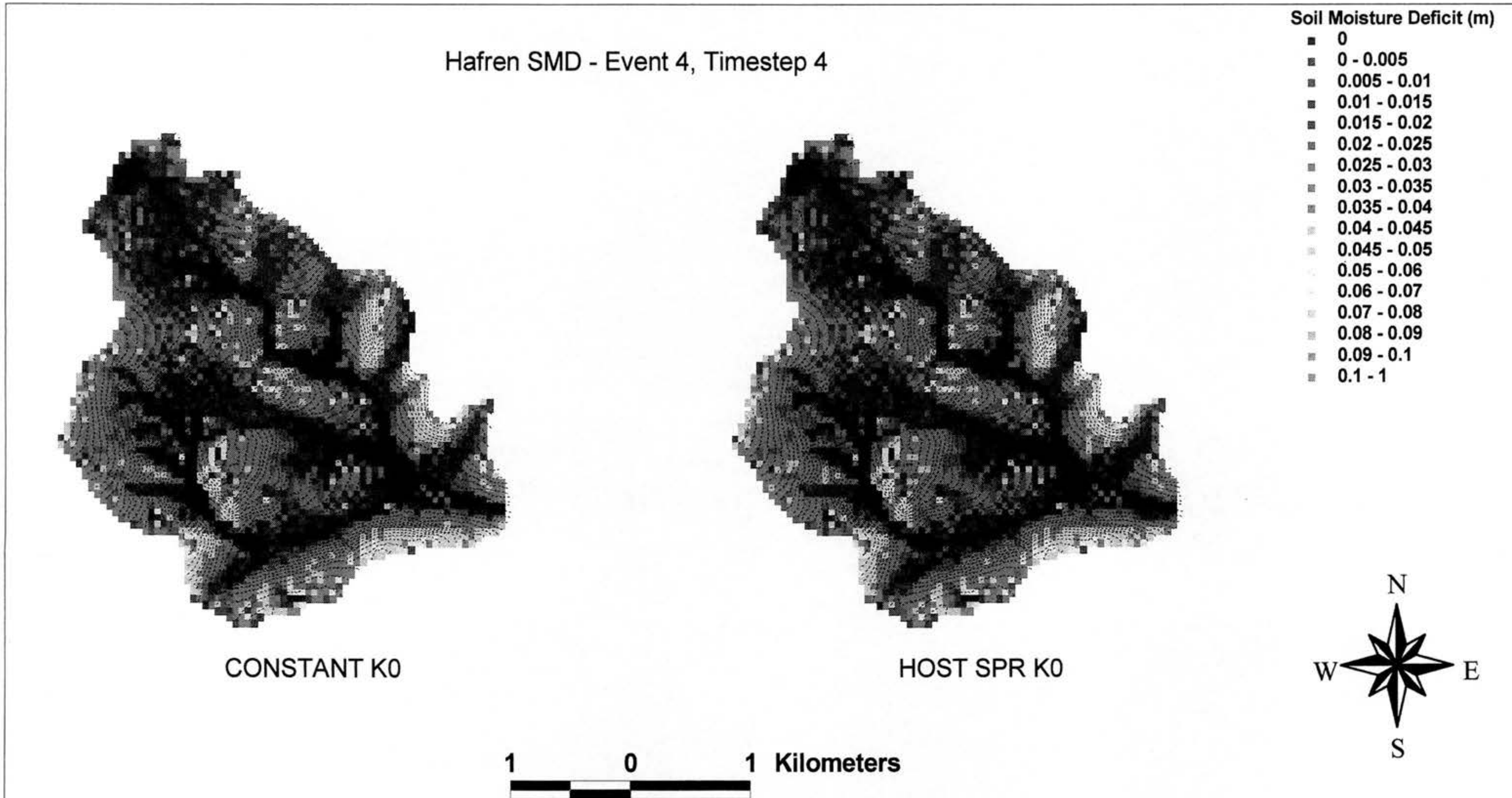

Hafren SMD - Event 3, Timestep 3
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers



Hafren SMD - Event 4, Timestep 1
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers


Hafren SMD - Event 4, Timestep 2
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

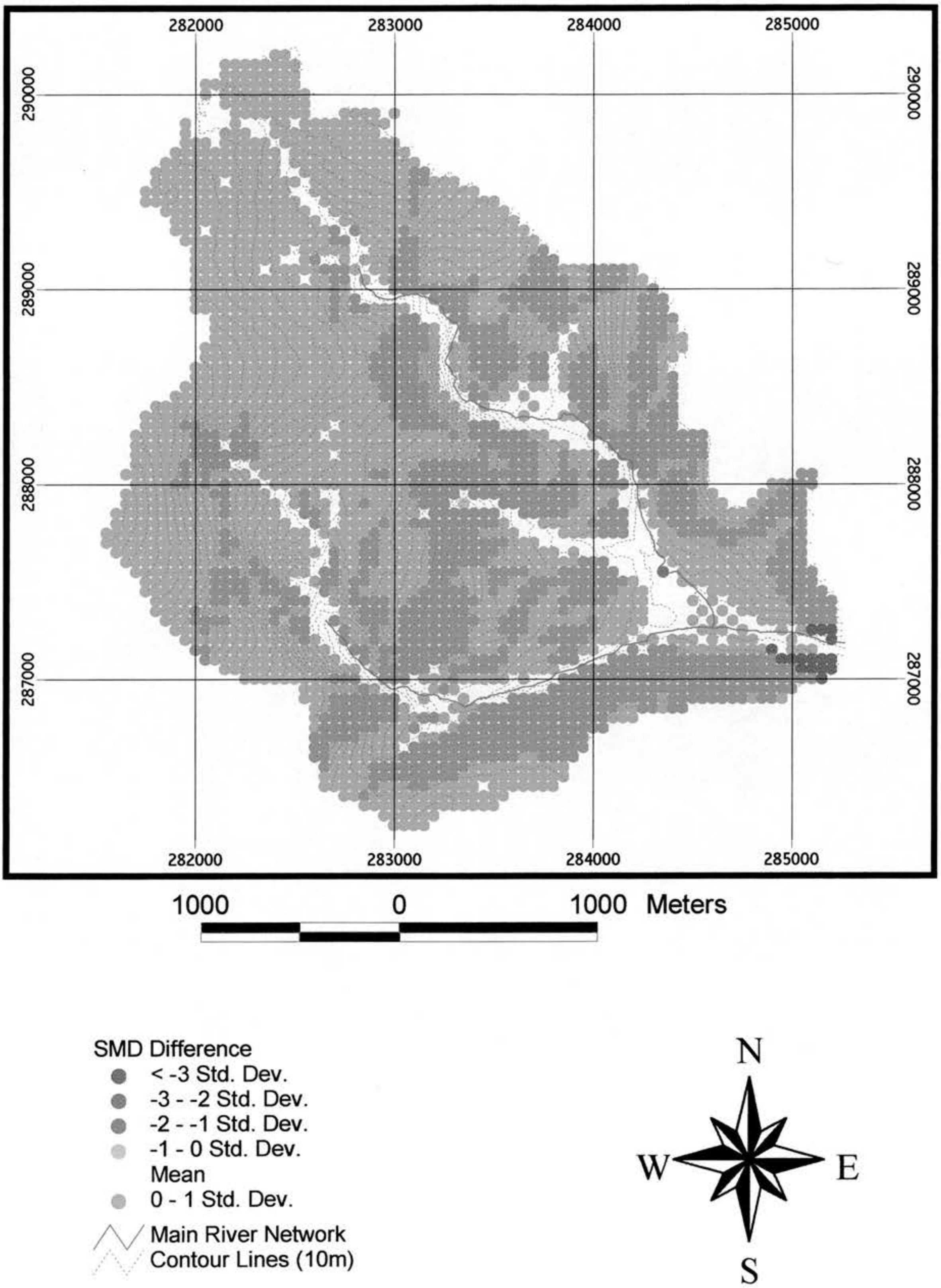

Hafren SMD - Event 4, Timestep 3
CONSTANT K0
HOST SPR K0
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
N
E
S
W
1
0
1
Kilometers


Hafren SMD - Event 4, Timestep 4
Soil Moisture Deficit (m)
0
0 - 0.005
0.005 - 0.01
0.01 - 0.015
0.015 - 0.02
0.02 - 0.025
0.025 - 0.03
0.03 - 0.035
0.035 - 0.04
0.04 - 0.045
0.045 - 0.05
0.05 - 0.06
0.06 - 0.07
0.07 - 0.08
0.08 - 0.09
0.09 - 0.1
0.1 - 1
CONSTANT K0
HOST SPR K0
N
W
E
S
1
0
1
Kilometers

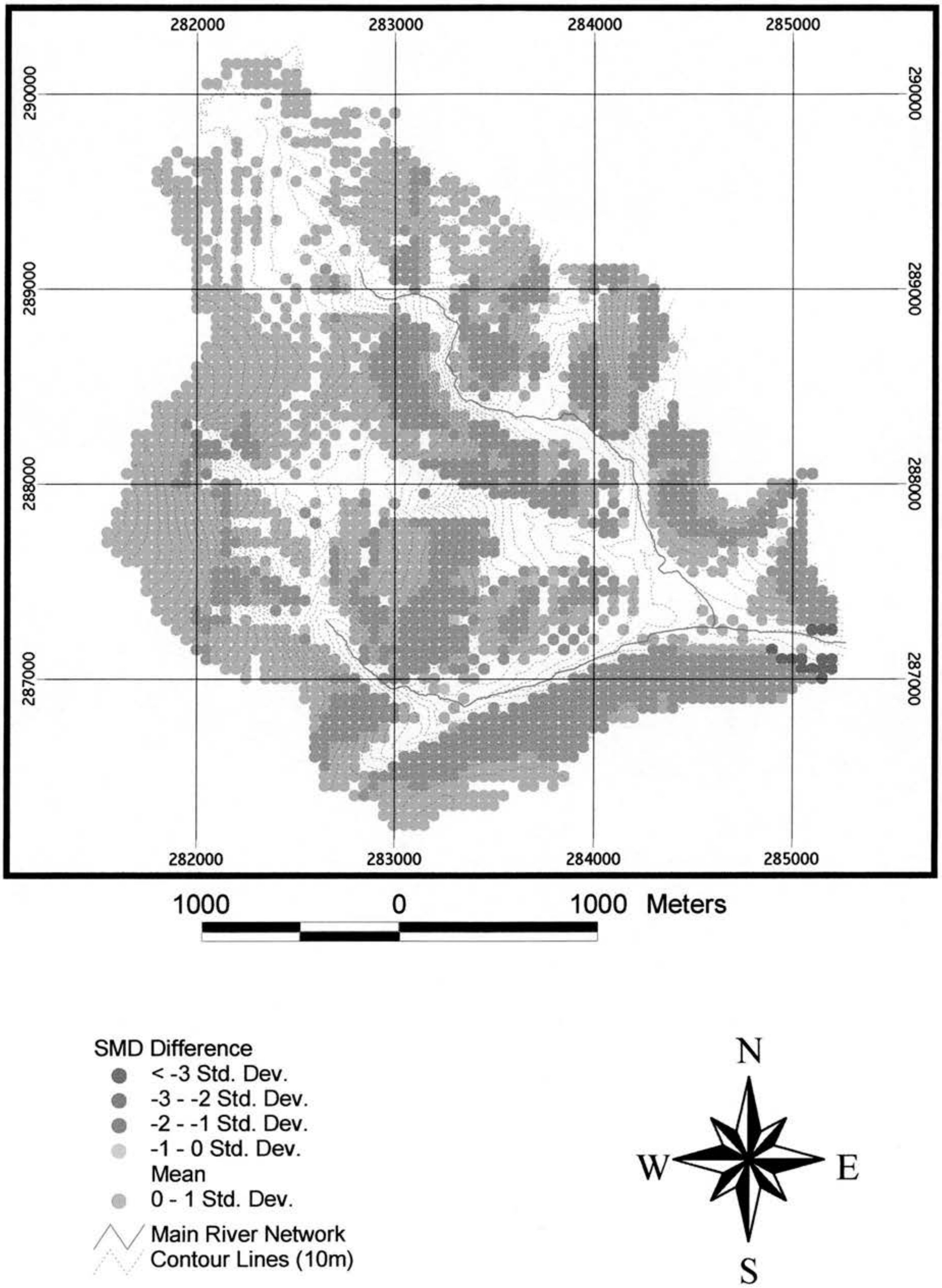
Appendix 3

Note for the Reader: Overhead transparency slides of the soil map and of the contour map have been placed in the back cover pocket to allow manual overlays with the maps in this Appendix.

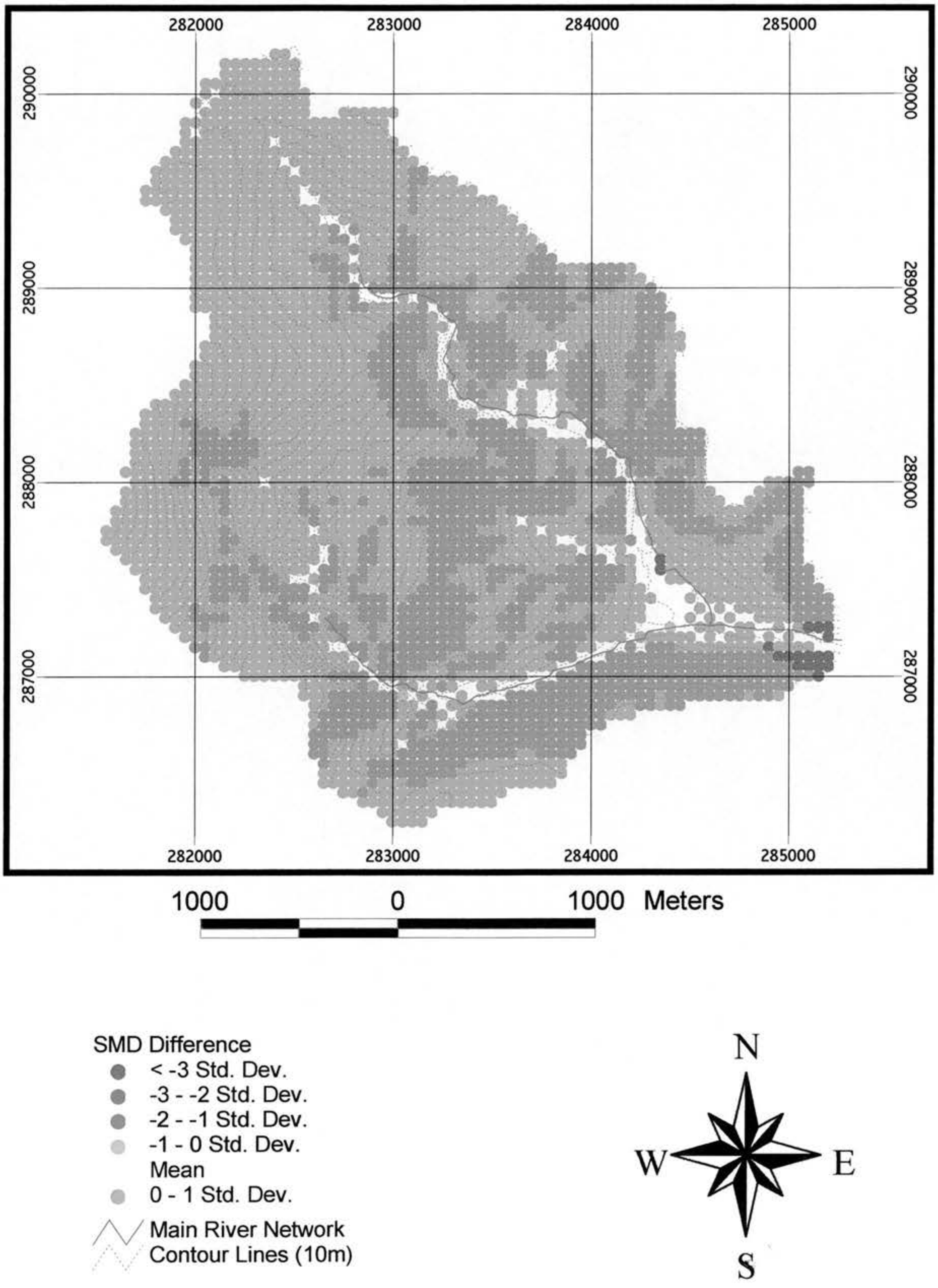
Hafren Event 1, Timestep 1
- SMD (HOST SPR K0 - Const. K0) -



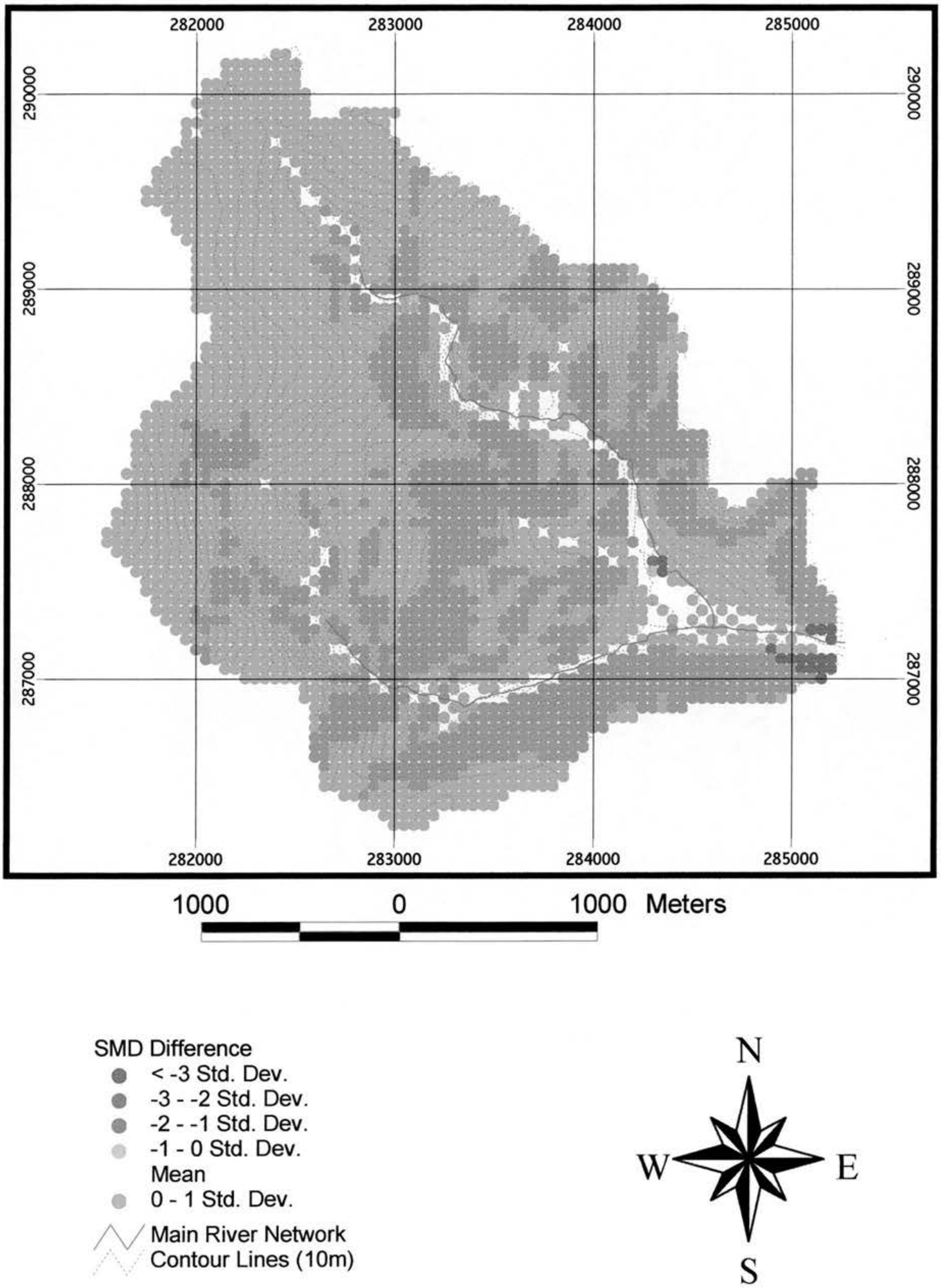
Hafren Event 1, Timestep 2
- SMD (HOST SPR K0 - Const. K0) -



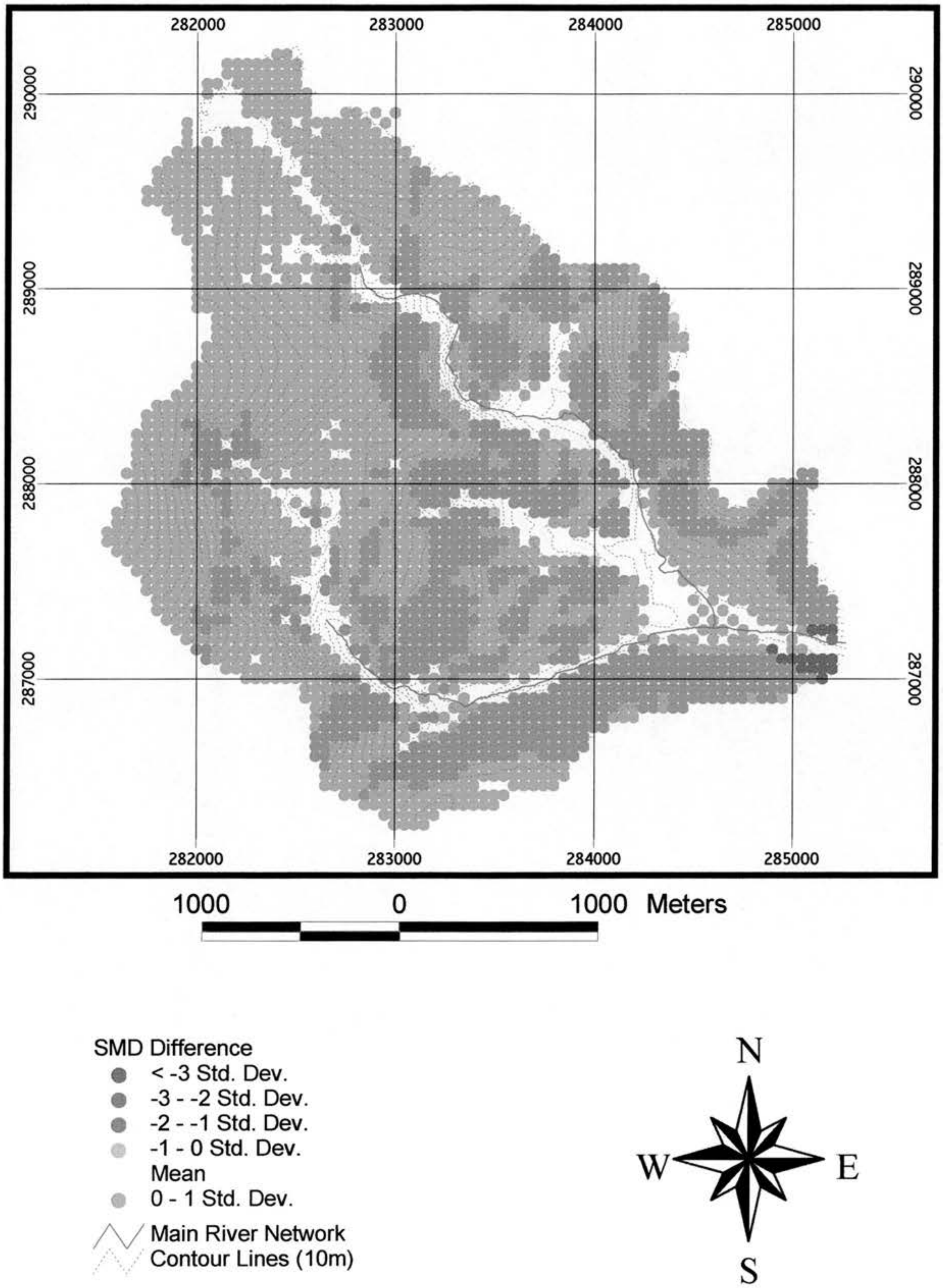
Hafren Event 1, Timestep 3
- SMD (HOST SPR K0 - Const. K0) -



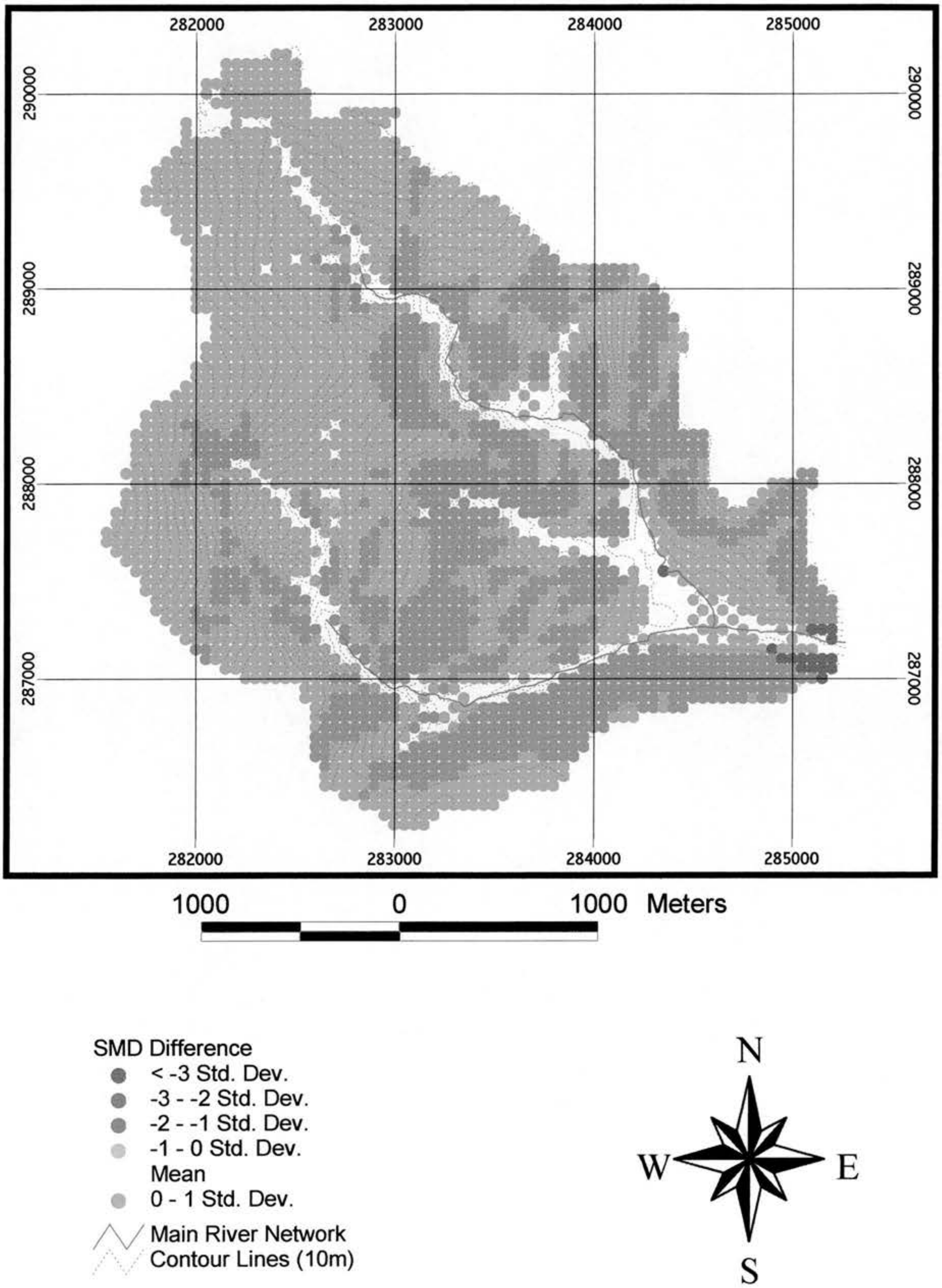
Hafren Event 2, Timestep 1
- SMD (HOST SPR K0 - Const. K0) -



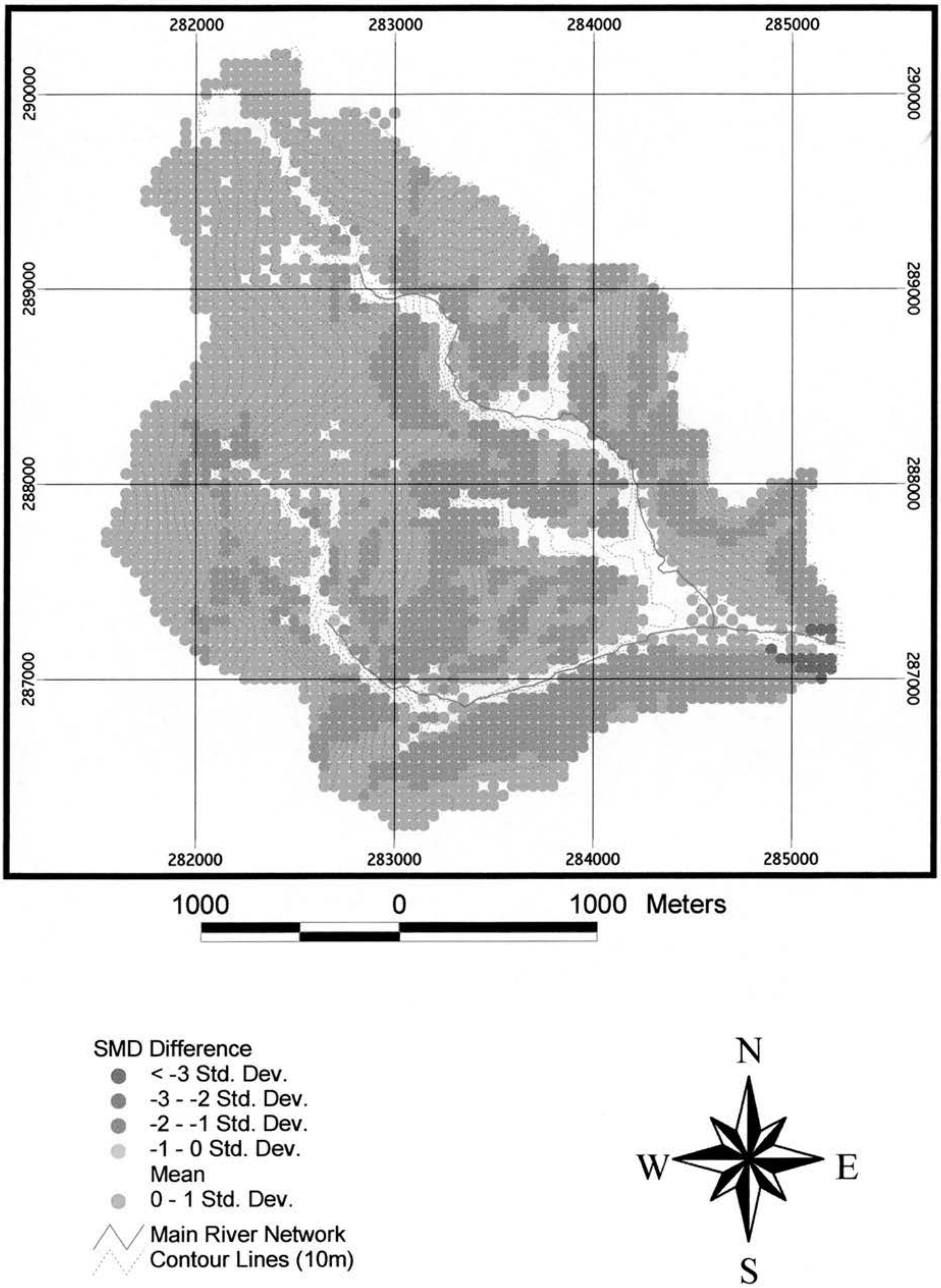
Hafren Event 2, Timestep 2
- SMD (HOST SPR K0 - Const. K0) -



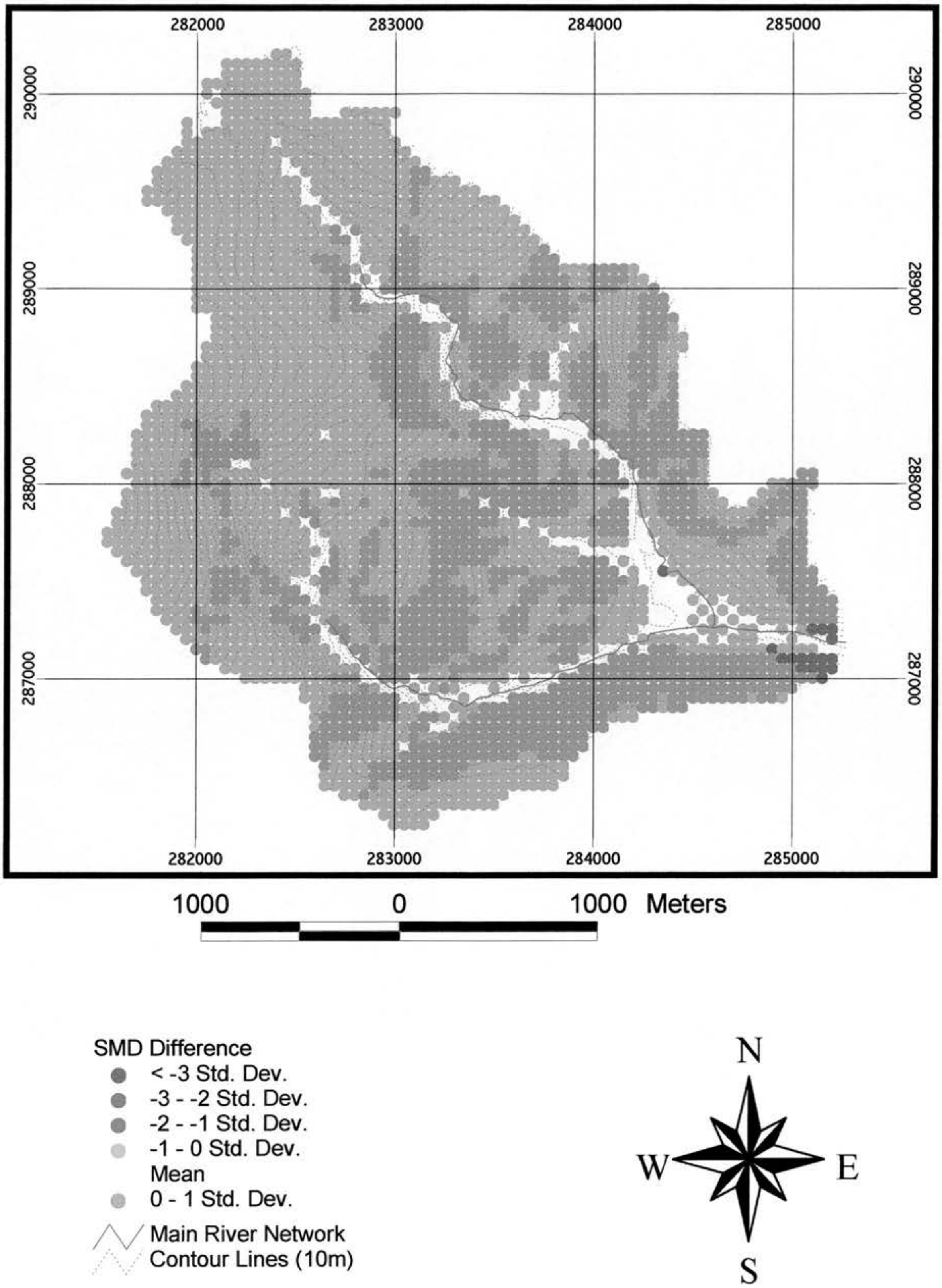
Hafren Event 2, Timestep 3
- SMD (HOST SPR K0 - Const. K0) -



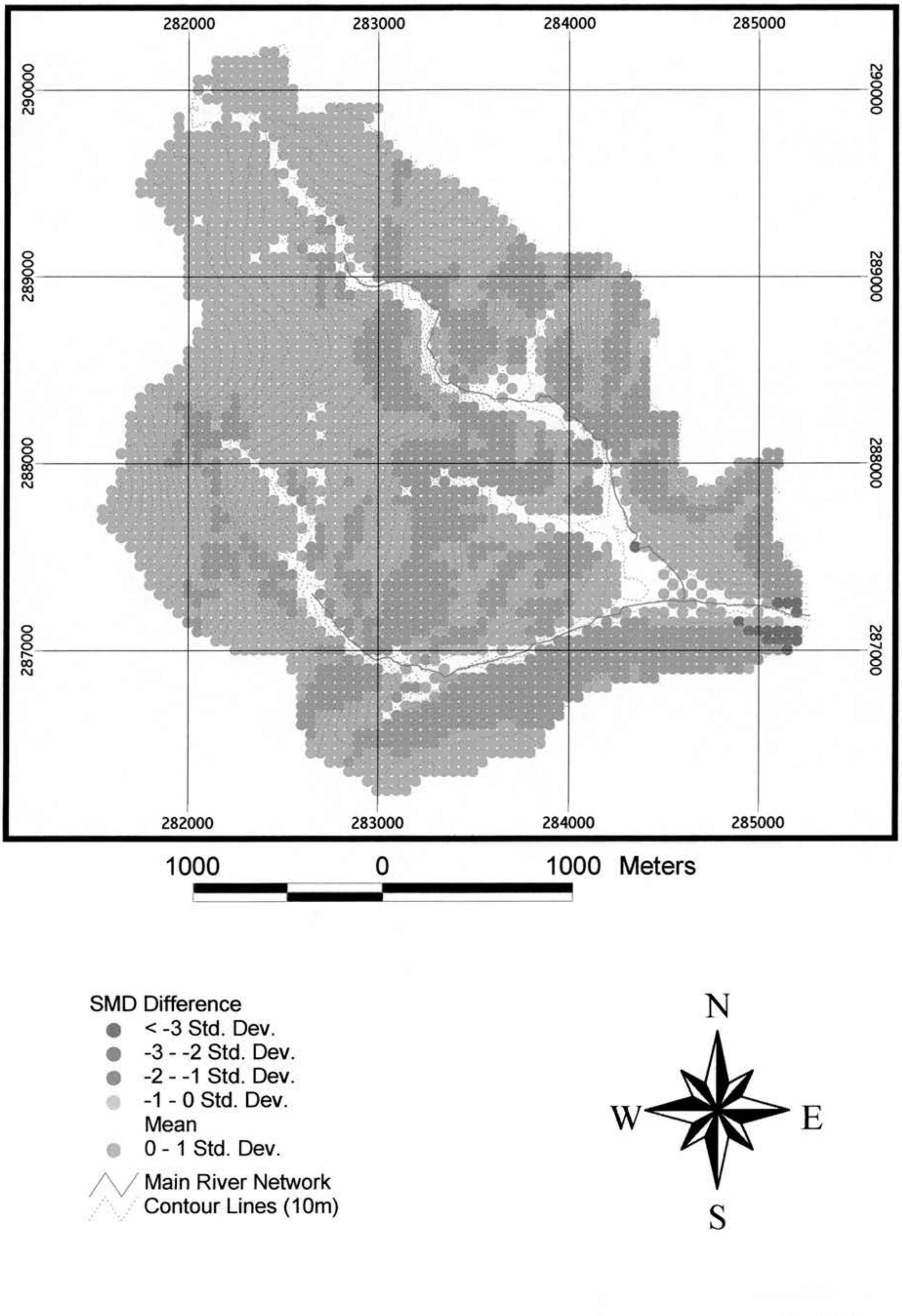
Hafren Event 2, Timestep 4
- SMD (HOST SPR K0 - Const. K0) -



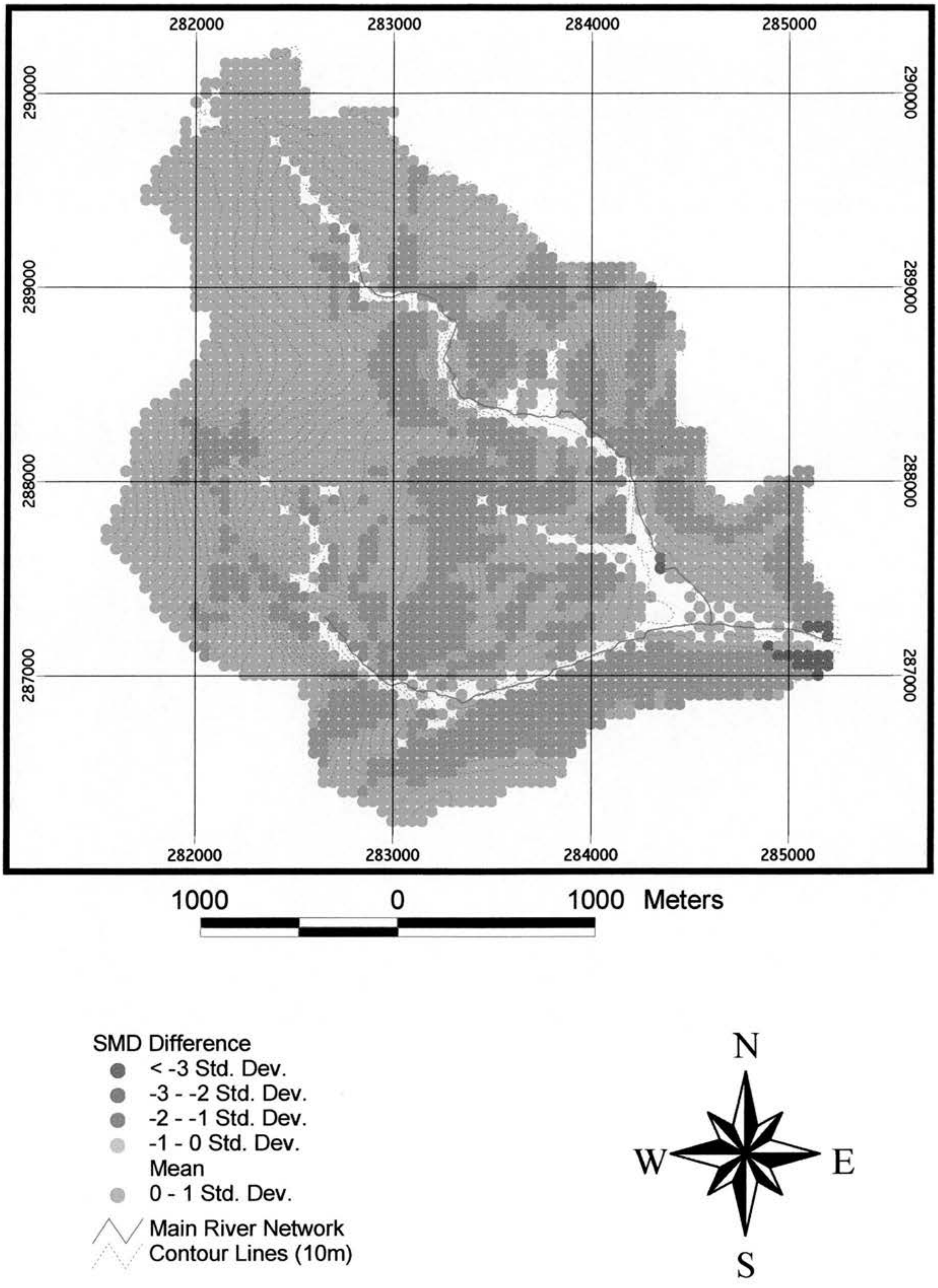
Hafren Event 2, Timestep 5
- SMD (HOST SPR K0 - Const. K0) -



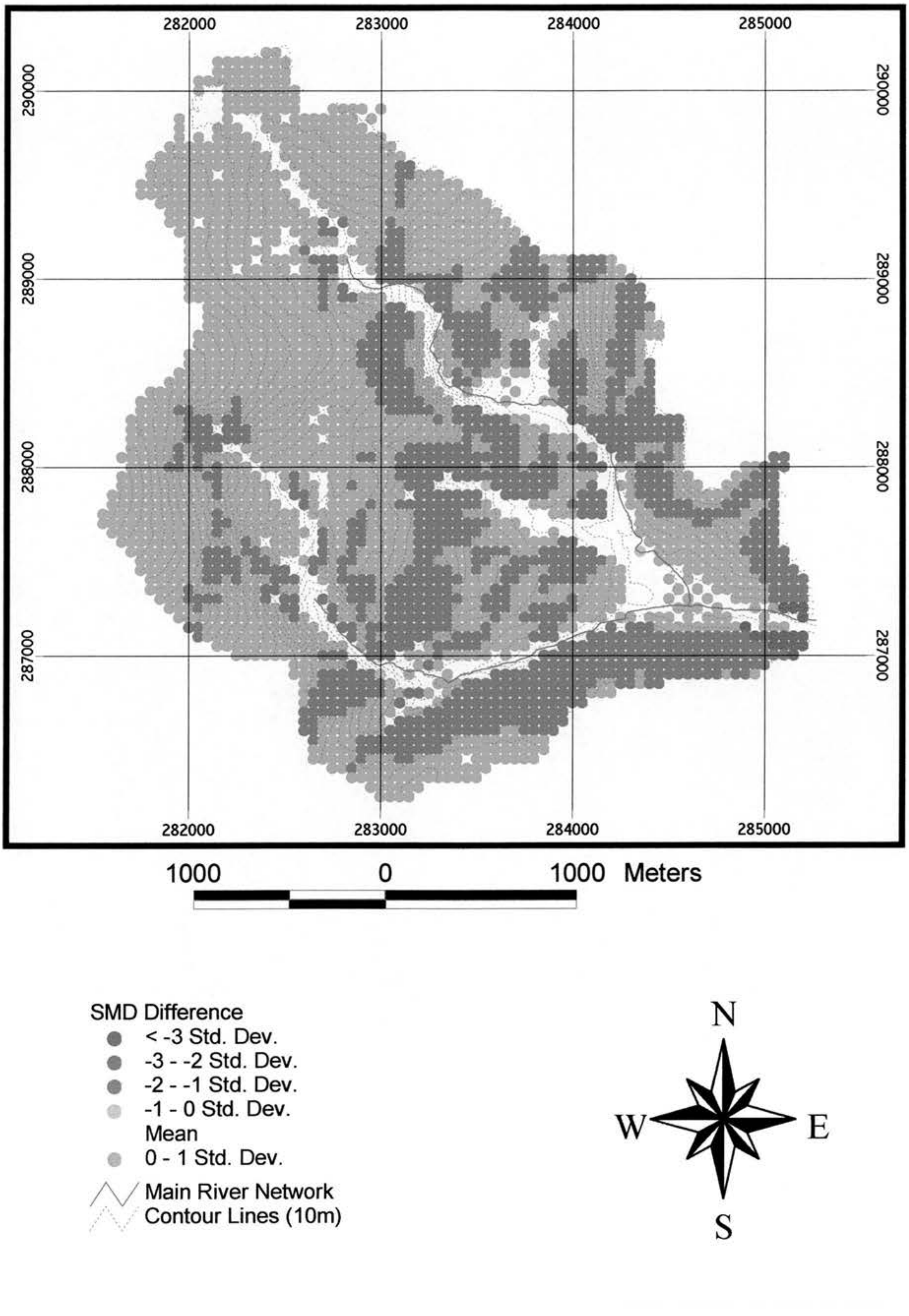
Hafren Event 2, Timestep 6
- SMD (HOST SPR K0 - Const. K0) -



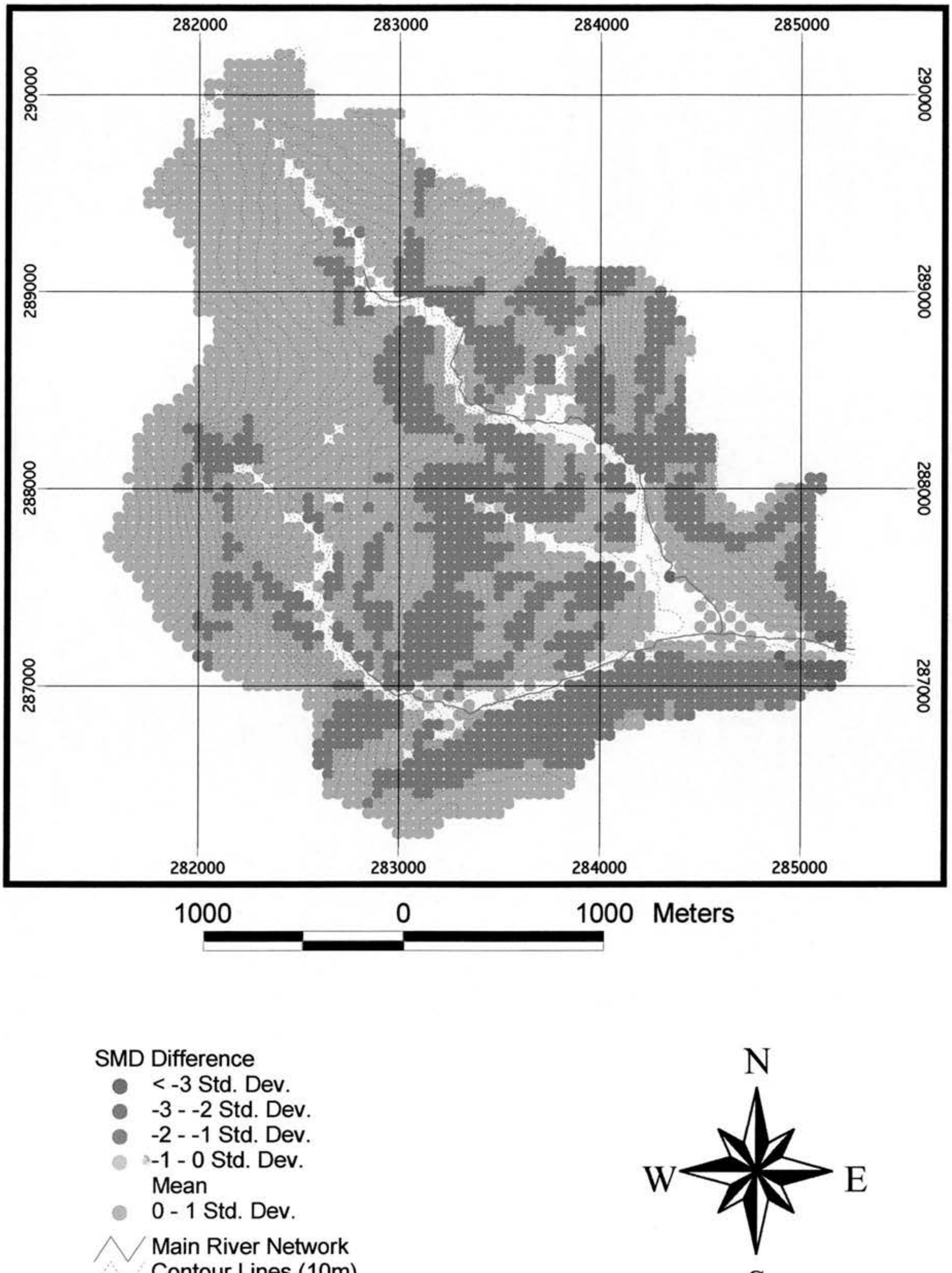
Hafren Event 3, Timestep 1
- SMD (HOST SPR K0 - Const. K0) -



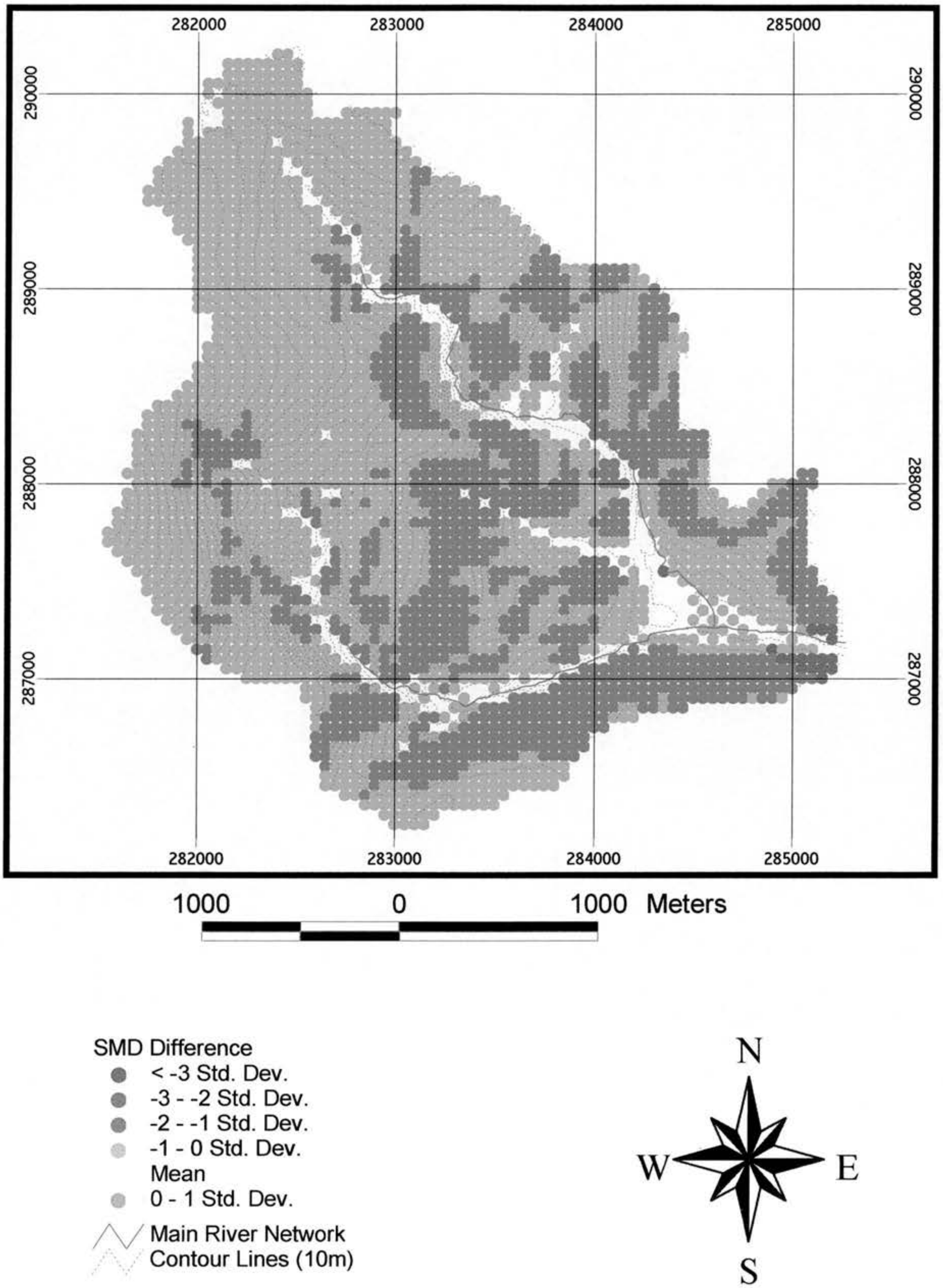
Hafren Event 3, Timestep 2
- SMD (HOST SPR K0 - Const. K0) -



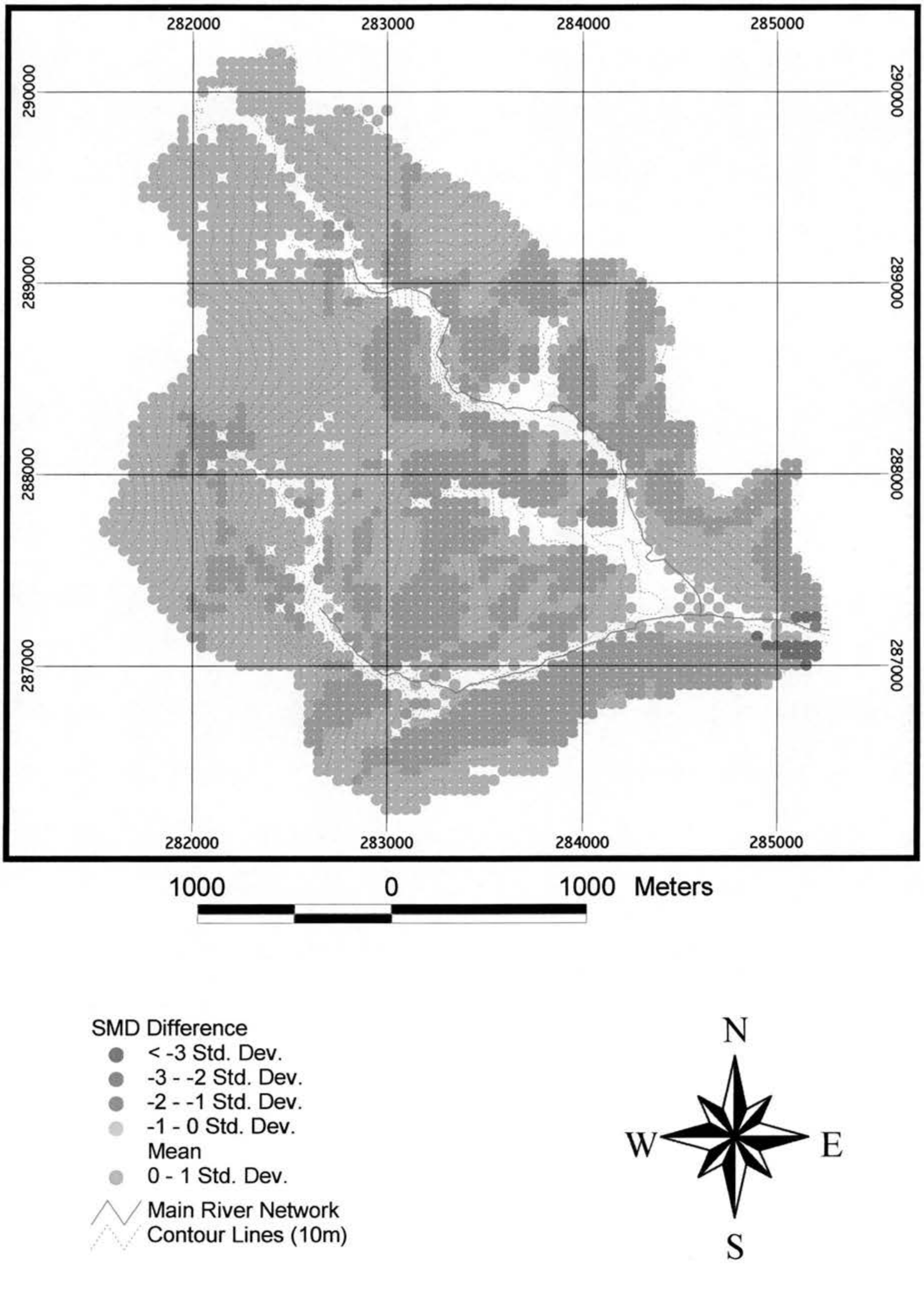
Hafren Event 3, Timestep 3
- SMD (HOST SPR K0 - Const. K0) -



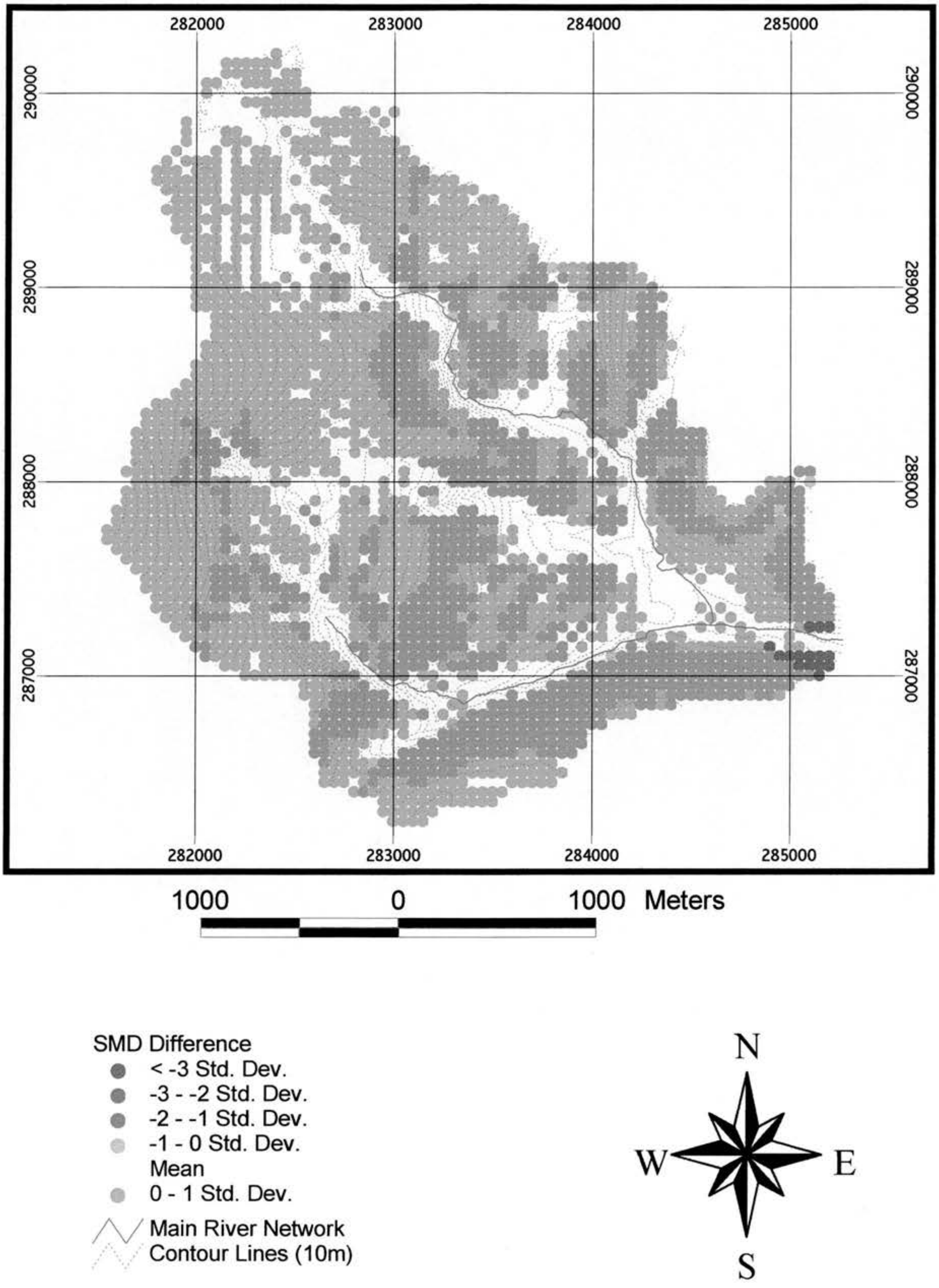
Hafren Event 4, Timestep 1
- SMD (HOST SPR K0 - Const. K0) -



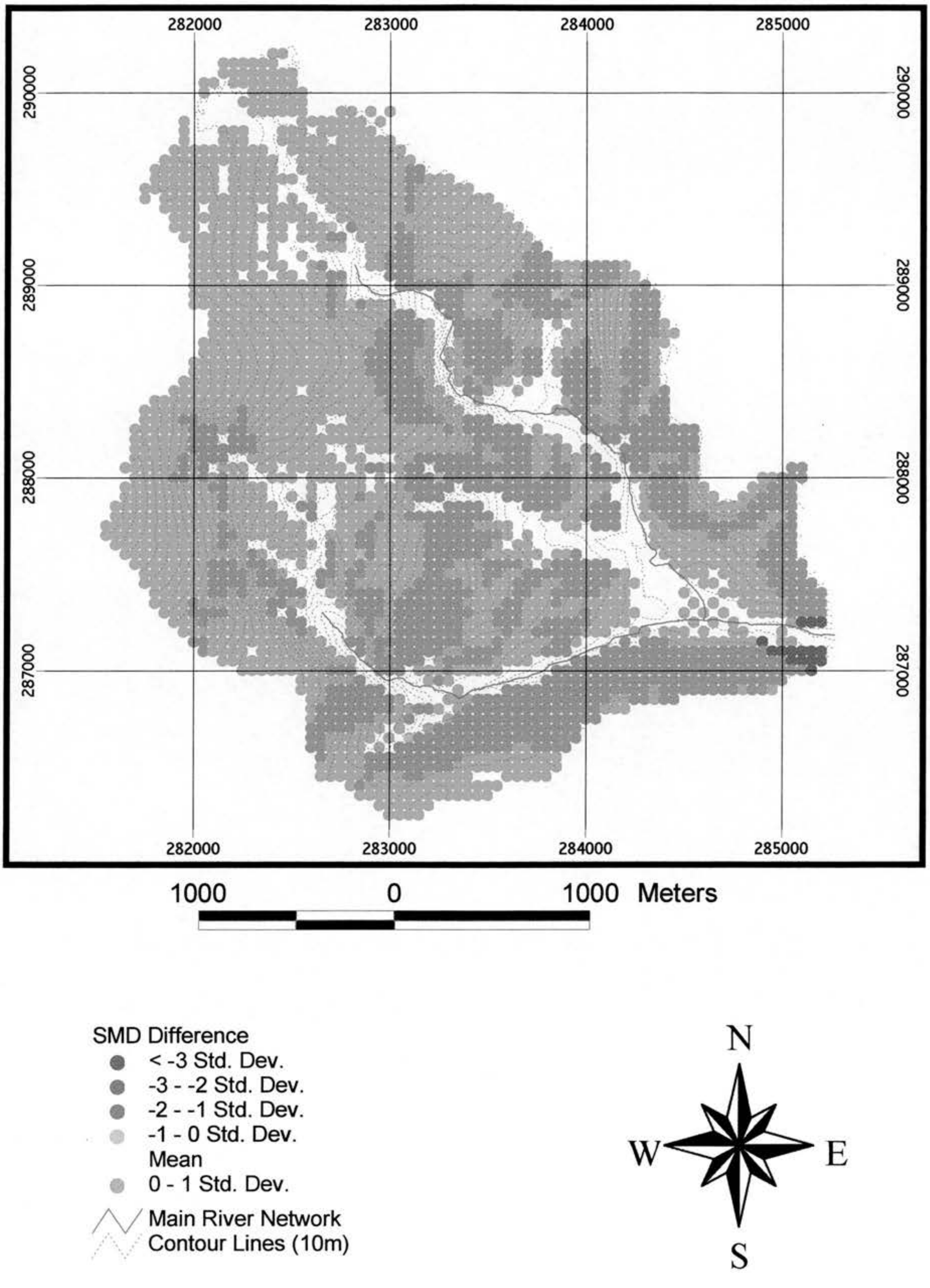
Hafren Event 4, Timestep 2
- SMD (HOST SPR K0 - Const. K0) -



Hafren Event 4, Timestep 3
- SMD (HOST SPR K0 - Const. K0) -

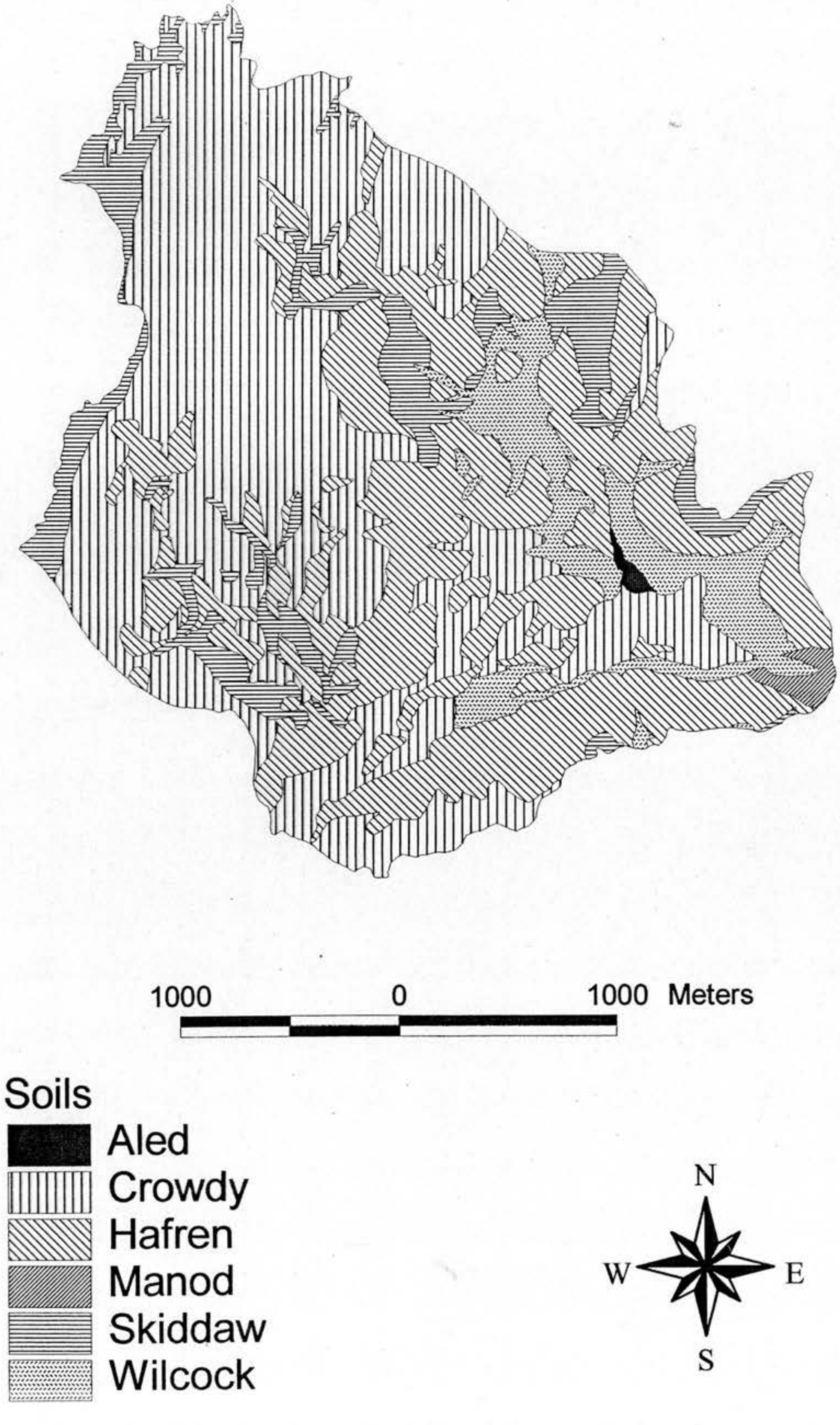


Hafren Event 4, Timestep 4
- SMD (HOST SPR K0 - Const. K0) -

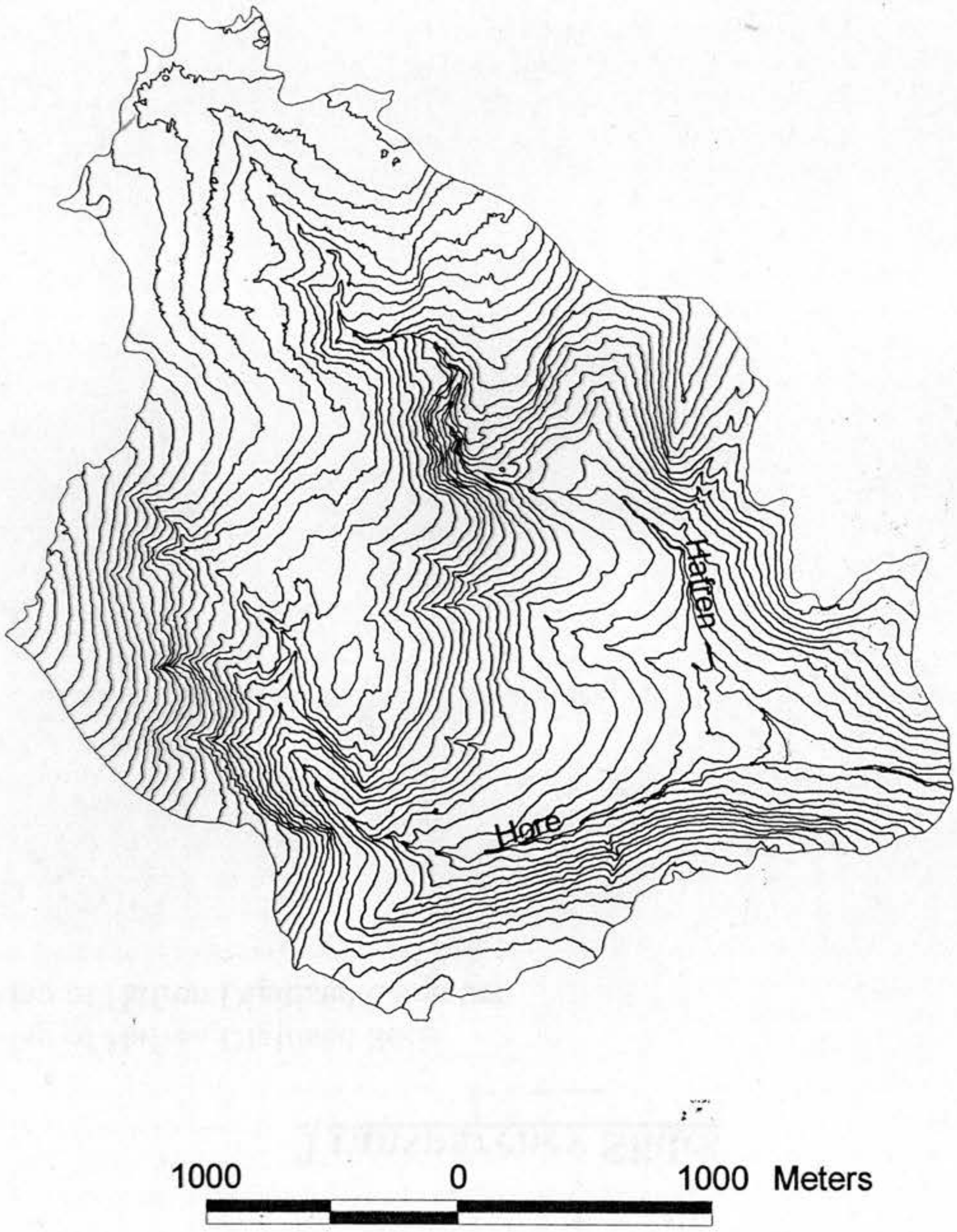


Transparency Slides

1) Map of Hafren Digitised Soils
2) Map of Hafren Digitised Contours



Hafren Digitised Soils



Hafren Digitised Contours